

UNIVERSITÁ DEGLI STUDI DI PAVIA

*Dipartimento di Fisica*

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# Introduction to Quantum Backflow

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## **Abstract**

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# Introduction

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## INTRODUCTION

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# Chapter 1

## Mathematical Tools

The aim of the first chapter is to introduce the theoretical set-up needed for our investigations. Here, we will outline the main mathematical tools and theorems that will be used in the study of quantum backflow. First of all, we will sum up the basic concepts of Hilbert spaces and the linear operators living on it. The second section will be entirely devoted to the introduction of the Fourier transform and of its properties which are essential in the study of kinematic aspects of particles. Last, we will focus on quantum mechanics summarizing the Schrödinger equation and the concept of observable as well as its connection with linear operators.

### 1.1 Hilbert Spaces and Operators

In quantum mechanics a wave function is a complex valued map  $\phi$  whose square of absolute value  $|\phi(x)|^2$  represents the distribution probability of finding the particle somewhere in the physical space. Generally, those functions are thought as elements of a particular vector space called Hilbert space. A complete definition of this important concept will be given in the following section.

First of all, we introduce a class of vector spaces in which we could define the "length" of a vector or the "distance" between two different vectors. Hence we have

**1.1.1 Definition (Normed vector space).** *Let  $V$  be a vector space in complex field.  $V$  is called normed space if there exists a map  $\|\cdot\| : V \rightarrow \mathbb{R}$  such that:*

$$(a) \quad \|v\| \geq 0 \quad \forall v \in V, \text{ and } \|v\| = 0 \text{ if and only if } v = 0$$

$$(b) \quad \|\alpha v\| = |\alpha| \|v\| \quad \forall \alpha \in \mathbb{C}, \quad \forall v \in V$$

$$(c) \quad \|v + w\| \leq \|v\| + \|w\| \quad \forall v, w \in V$$

and this map  $\|\cdot\|$  is called norm of the space  $V$ .

**1.1.2 Example.** Consider the vector space  $\mathbb{C}^n$  with the norm defined by  $\|z\| = \left[ \sum_{i=1}^n |z_i|^2 \right]^{\frac{1}{2}}$ , where  $z = (z_1, \dots, z_n) \in \mathbb{C}^n$ . This is a normed space.

The definition of norm naturally introduce a concept of convergence in such vector space. In fact, we can define that a certain sequence  $\{v_n\} \in V$  converges to a vector  $v \in V$  if  $\lim_{n \rightarrow \infty} \|v_n - v\| = 0$ .

A well-known fact from theory on  $\mathbb{R}^n$  is that convergent sequences  $\{v_n\}_{n \in \mathbb{N}}$  in a normed space  $V$  satisfy the *Cauchy property* (see [1, Chap. 2]):

**1.1.3 Definition (Cauchy sequences).** A sequence  $\{v_n\}_{n \in \mathbb{N}}$  in a normed space  $V$  is called a *Cauchy sequence* if, for any  $\varepsilon > 0$ , there exists  $N_\varepsilon \in \mathbb{R}$  such that  $\|v_n - v_m\| < \varepsilon$  whenever  $n, m > N_\varepsilon$ .

Now, we introduce the concept of *complete normed space*.

**1.1.4 Definition (Banach spaces).** A normed space is called a *Banach space* if it is complete, i.e. if any Cauchy sequence inside the space converges to a point of the space.

Now, we want to identify Hilbert spaces. In this new class of vector spaces we will be able to define the fundamental concept of scalar product.

**1.1.5 Definition (Hilbert space).** Let  $\mathcal{H}$  be a vector space over the complex field.  $\mathcal{H}$  is a *Hilbert space* if there exists a map  $(\cdot|\cdot) : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{C}$  (called *scalar product*) such that:

- (a)  $(w|\alpha v_1 + \beta v_2) = \alpha(w|v_1) + \beta(w|v_2) \quad \forall w, v_1, v_2 \in \mathcal{H}, \forall \alpha, \beta \in \mathbb{C}$
- (b)  $(w|v) = \overline{(v|w)} \quad \forall v, w \in \mathcal{H}$
- (c)  $(v|v) \geq 0 \quad \forall v \in \mathcal{H}$  and  $(v|v) = 0$  if and only if  $v = 0$

and if  $\mathcal{H}$  is complete with the norm defined by  $\sqrt{(\cdot|\cdot)}$ .

**1.1.6 Example.** (a)  $\mathbb{C}^n$  with the inner product  $(u|v) := \sum_{i=1}^n \overline{u_i} v_i$ , where  $u = (u_1, \dots, u_n)$ ,  $v = (v_1, \dots, v_n)$ , is a Hilbert space.

(b) Consider the set

$$L := \left\{ f : \mathbb{R}^n \rightarrow \mathbb{C} \mid \int_{\mathbb{R}^n} |f(x)|^2 dx < \infty \right\} \quad (1.1)$$

and the equivalence class  $[f]$  of a function  $f \in L$ :

$$[f] = \{g \in L \mid f = g \text{ almost everywhere}\}. \quad (1.2)$$

Then, we define the space  $L^2(\mathbb{R}^n)$  as

$$L^2(\mathbb{R}^n) = \{[f] \mid f \in L\}. \quad (1.3)$$

$L^2(\mathbb{R}^n)$  is a Hilbert space with the scalar product defined by:

$$([f]|[g]) = \int_{\mathbb{R}^n} \overline{f(x)} g(x) dx. \quad (1.4)$$

This space play a key role in quantum mechanics. In fact each wave function  $\phi$  is considered as an element of this space such  $\int_{\mathbb{R}^n} |\phi(x)|^2 dx = 1$ .<sup>1</sup>

Now we enunciate some notable definitions and results concerning the linear operators on normed and Hilbert spaces.

**1.1.7 Definition.** Let  $V$  and  $V'$  be normed spaces. A linear map  $T : D(T) \rightarrow V'$ , where  $D(T) \subseteq V$  is a subspace of  $V$ , is called a **linear operator**. Furthermore,

- (a) if  $D(T)$  is dense in  $V$ ,  $T$  is called a **dense operator**.<sup>2</sup>

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<sup>1</sup>Hereafter, we shall write  $f$  instead of  $[f]$ .

<sup>2</sup> $D(T)$  is dense in  $V$  when for all  $v \in V$  there exists a sequence  $\{v_n\} \in D(T)$  converging to  $v$ .

- (b) The set  $\{Tv \mid v \in D(T)\}$  it is called **Range** of the operator  $T$  and it is indicated with the symbol  $Ran(A)$ .
- (c) The set  $\{v \in D(T) \mid Tv = 0\}$  it is called **Kernel** of the operator  $T$  and it is indicated with the symbol  $Ker(A)$ .
- (d)  $T$  is a **closed** operator if its graph  $G(T) := \{(v, Tv) \in V \times V' \mid v \in D(T)\}$  is a closed set. Instead  $T$  is a **closable** operator if there exists a closed extension of  $T$  (called  $\bar{T}$ ).
- (e) An operator  $T : V \rightarrow V'$  is **bounded** if  $\exists k \in (0, +\infty)$  such that

$$\|Tv\| \leq k\|v\| \quad \forall v \in V \quad (1.5)$$

or equivalently,

$$\|T\| := \sup_{\|v\|=1} \|Tv\| < +\infty \quad (1.6)$$

We represent the set of linear operators from  $V$  to  $V'$  with the symbol  $\mathcal{L}(V, V')$  while bounded operators are indicated with  $\mathcal{B}(V, V')$ .

**1.1.8 Observation.** The basic property of bounded operators is that for any bounded subset of the domain  $V$  its image remains bounded. Furthermore, we prove that  $\mathcal{B}(V)$  is also a normed space with the definition of norm given in Eq. (1.6).

**1.1.9 Example.** Consider the Hilbert space  $L^2(\mathbb{R})$  and the derivative operator  $P := -i\partial_x$  (called the *momentum* operator).  $P$  could not be defined for all the elements in  $L^2(\mathbb{R})$ . But it is well defined in the space of test-functions  $C_0^\infty(\mathbb{R})$ , which is a closed subspace of  $L^2(\mathbb{R})$ . Other examples of dense operators in  $L^2(\mathbb{R})$  are the multiplication operator  $X := x$  (called *position* operator) and  $P^2 := -\partial_x^2$ . All these operators will be investigated more in detail in the third part of the chapter.

**1.1.10 Theorem.** Let be  $V$  and  $V'$  two normed space and  $T : V \rightarrow V'$  a linear operator. Then the following statements are equivalent:

- (a)  $T \in \mathcal{B}(V, V')$
- (b)  $T$  is continuous,
- (c)  $T$  is continuous in 0.

A proof of this theorem could be found in [1, Th. 2.43].

Another fundamental concept is that of *adjoint operator*. It is common to have to deal with the scalar product of a vector and the image of another vector under a linear operator. Take for example a linear operator  $T : D(T) \rightarrow \mathcal{H}'$  and consider the scalar product:

$$(w|Tv) \text{ with } v \in D(T) \subseteq \mathcal{H}, \quad w \in \mathcal{H}'. \quad (1.7)$$

We want to ask ourself if there exists a particular operator  $T^*$  defined in some subspace  $D(T^*)$  such that

$$(T^*w|v) \quad \forall w \in D(T^*), v \in D(T) \quad (1.8)$$

More generally, we may think about the first scalar product as a linear functional  $f_T : D(T) \rightarrow \mathbb{C}$  which map  $v \mapsto f_T(v) := (w|Tv)$  and we ask whether there exists a particular vector  $w_f$  which *represents* our functional, i.e.  $f_T(v) = (w^*|v)$ . Here  $w^*$  has the same role of  $T^*w$  in the previous equation. In order to investigate  $\omega$  existence:

**1.1.11 Proposition (Existence of adjoint operator).** *If  $\mathcal{H}$  and  $\mathcal{H}'$  are Hilbert spaces and  $T \in \mathcal{B}(\mathcal{H}, \mathcal{H}')$ , then there exists a unique adjoint operator  $T^* \in \mathcal{B}(\mathcal{H}', \mathcal{H})$  such that*

$$(w|Tv) = (T^*w|v) \quad \forall w \in \mathcal{H}', \quad \forall v \in \mathcal{H}. \quad (1.9)$$

The existence of  $T^*$  is a consequence of the *Riesz's representation theorem* and a complete proof of the equivalence and of the other points above could be found on [1, Ch. 2-3].

Now, we classify different types of bounded operators.

**1.1.12 Definition.** *Let  $\mathcal{H}$  and  $\mathcal{H}'$  be Hilbert spaces.*

- (a)  $T \in \mathcal{B}(\mathcal{H})$  is **self-adjoint** if  $T = T^*$ .
- (b)  $T \in \mathcal{L}(\mathcal{H}, \mathcal{H}')$  is **isometric** if  $(Tv|Tw) = (v|w)$  for all  $v, w \in \mathcal{H}$ , or equivalently if  $T \in \mathcal{B}(\mathcal{H}, \mathcal{H}')$  and  $T^*T = \mathbb{I}_{\mathcal{H}}$ .
- (c)  $T \in \mathcal{L}(\mathcal{H}, \mathcal{H}')$  is **unitary** if it is isometric and surjective, or equivalently if  $T \in \mathcal{B}(\mathcal{H}, \mathcal{H}')$ ,  $T^*T = \mathbb{I}_{\mathcal{H}}$  and  $TT^* = \mathbb{I}_{\mathcal{H}'}$ .
- (d)  $T \in \mathcal{L}(\mathcal{H}, \mathcal{H})$  is **positive** if  $(v|Tv) \geq 0$  for all  $v \in \mathcal{H}$ .<sup>3</sup>

Now, we consider the set of all dense operators. In particular, we want to study the existence of an adjoint for these operators. In this case, the scenario is more complicated. The problem is that the choice of  $T^*w$  as in the equation (1.8) could not be unique, and an adjoint operator could not be defined at all. In fact, if we take a vector  $T^*w$  such that equation (1.8) holds for any  $v \in D(T)$ , and sum  $v_0 \in D(T)^\perp$ , the equation still holds true and  $T^*$  could not be a function. In order to avoid this problem defining  $T^*$ , we need to impose our operators to be at least dense so that  $D(T)^\perp = \emptyset$ . In this case:

**1.1.13 Definition.** *Let  $\mathcal{H}$  a Hilbert space, and  $T : D(T) \rightarrow \mathcal{H}$  a dense operator. Then we call the adjoint operator  $T^*$  the operator defined in*

$$D(T^*) = \{v \in \mathcal{H} \mid \exists z_{T,v} \in \mathcal{H} \text{ such that } (v|Tw) = (z_{T,v}|w) \quad \forall w \in D(T)\}, \quad (1.10)$$

and which maps  $v \mapsto T^*v := z_{T,v}$ . Furthermore,  $T$  is

- (a) **Hermitian** if  $\forall v, w \in D(T)$  we have  $(v|Tw) = (Tv|w)$ ,
- (b) **symmetric** if it is Hermitian and  $D(T)$  is dense,
- (c) **self-adjoint** if it is symmetric and  $T = T^*$ ,
- (d) **essentially self-adjoint** if  $D(T)$  and  $D(T^*)$  are dense and  $T^* = T^{**}$ ,
- (e) **normal** if  $T^*T = TT^*$  in their standard domain.

**1.1.14 Example.** Let us consider the momentum operator  $P := -i\partial_x$  as Example 1.1.9. As we said before,  $P$  is dense since we could define it over the dense subspace of smooth functions with compact support  $C_0^\infty(\mathbb{R})$ . Using integration by parts it holds that  $\forall f, g \in C_0^\infty(\mathbb{R})$   $(f| -i\partial_x g) = (-i\partial_x f|g)$ . Then  $P$  is Hermitian as well.

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<sup>3</sup>Generally, a positive operator is indicated with " $T \geq 0$ "

The next concept we have to describe is that of *spectrum* of a linear operator. It is assumed in quantum mechanics that the possible results of a measurement are given by the "eigenvalues" of suitable linear operators. We define the spectrum as the complement of another set of complex numbers called *resolvent set*.

**1.1.15 Definition (Resolvent and Spectrum).** Let  $T$  be an operator in a normed space  $X$ .

(a) The resolvent set of  $T$  is the set  $\rho(T)$  containing the values  $\lambda \in \mathbb{C}$  such that:

- (i)  $\overline{\text{Ran}(T - \lambda\mathbb{I})} = X$ ,
- (ii)  $(T - \lambda\mathbb{I}) : D(T) \rightarrow X$  is injective,
- (iii)  $(T - \lambda\mathbb{I})^{-1} : \text{Ran}(T - \lambda\mathbb{I}) \rightarrow X$  is bounded.

(b) The spectrum of  $T$  is the set  $\sigma(T) := \mathbb{C} \setminus \rho(T)$ .

It is the union of the following three sets:

- (i) the point spectrum of  $A$ ,  $\sigma_p(A)$ , containing all those  $\lambda \in \mathbb{C}$  such that  $A - \lambda\mathbb{I}$  is not injective,
- (ii) the continuous spectrum,  $\sigma_c(A)$ , containing all those  $\lambda \in \mathbb{C}$  such that  $A - \lambda\mathbb{I}$  is still injective and the identity  $\overline{\text{Ran}(A - \lambda\mathbb{I})} = X$ , but  $(A - \lambda\mathbb{I})^{-1}$  is not bounded,
- (iii) the residual spectrum,  $\sigma_r(A)$ , containing all those  $\lambda \in \mathbb{C}$  such that  $A - \lambda\mathbb{I}$  is not injective, but  $\overline{\text{Ran}(A - \lambda\mathbb{I})} \neq X$ .

Note that from this definition the spectrum has a more complicated structure than the simple set of all those numbers  $\lambda$  such that there exists a solution  $v$  for the equation  $Av = \lambda v$  (the only point spectrum  $\sigma_p(A)$ ).

In our dissertation, the following relation between self-adjointed operators and their spectrum will be useful.

**1.1.16 Proposition.** Consider Hilbert space  $\mathcal{H}$  and  $T \in \mathcal{B}(\mathcal{H})$ . Then, the relation  $\sigma(T) \subseteq [-\|T\|, \|T\|]$  holds. Furthermore, if  $T = T^*$  we have

- (a)  $\sigma(T) \subset [m, M]$ , where  $m = \inf_{\|v\|=1} (v|Tv)$  and  $M = \sup_{\|v\|=1} (v|Tv)$ ,
- (b)  $m, M \in \sigma(T)$ ,
- (c)  $\|T\| = \max\{-m, M\}$ .

Before passing to the next argument, we have to introduce a final concept: *projectors operator*. We will see that calculating the probability of some outcome from a certain measure implies the projecting of some vector  $v$  into a closed subspace of a Hilbert space (i.e. the eigenspace of a linear operator associated with an eigenvalue  $\lambda$ ). Hence we define:

**1.1.17 Definition (Projector operator).** Let  $\mathcal{H}$  and  $P \in \mathcal{B}(\mathcal{H})$  a bounded operator.  $P$  is called an orthogonal projector if  $P^2 = P$  and  $P = P^*$ .

Here with the condition  $P^2 = P$  we are considering that once we have projected a vector into some subspace, applying again the same projection doesn't modify the vector anymore. Furthermore it could be proved (see [1, Prop. 3.53]) that for each projector  $P$  there exists a closed subspace  $W \subseteq \mathcal{H}$  such that  $P$  acts on some vector  $v \in \mathcal{H}$  just by projecting him into  $W$ .

Once we have given this other definition, we are able to pass at the next argument this chapter.

## 1.2 Fourier Transform

The second part of this section will be dedicated to the concept of *Fourier transformation*. It is known that if we take a real function  $f$  defined in some interval it could be decomposed as an infinite sum of trigonometric function (called the Fourier series), unless  $f$  breaks some necessary hypothesis. In general, for functions defined in  $\mathbb{R}$  (i.e.  $L^2(\mathbb{R})$ ) things are more complicated but we are able to write a decomposition on the space of frequencies. In this case we will no longer have an infinite countable sum, but we have to integrate all the *frequencies* over  $\mathbb{R}$ . The function defined by all these frequencies components is called the Fourier transform of our function. But before to arrive at the rigorous definition we need to do a necessary preamble. Then, we start with the following definition:

**1.2.1 Definition (Schwartz test function).** Let  $f : \mathbb{R} \rightarrow \mathbb{C}$  a smooth function. Then,  $f$  is called a *Schwartz test function* (or *rapidly decreasing functions*) if for all  $\alpha, \beta \in \mathbb{N}$  we have  $\|f\|_{\alpha, \beta} := \sup_{x \in \mathbb{R}} |x^\alpha \partial_x^\beta f(x)| < +\infty$ . This class of function is indicated with the symbol  $\mathcal{S}(\mathbb{R})$ . Furthermore, we said that a sequence  $\{f_n\} \in \mathcal{S}(\mathbb{R})$  converge in  $\mathcal{S}(\mathbb{R})$  if there exists a function  $f \in \mathcal{S}(\mathbb{R})$  such that for all  $\alpha, \beta \in \mathbb{N}$  we have  $\lim_{n \rightarrow \infty} \|f_n - f\|_{\alpha, \beta} = 0$ . In this case we write  $f_n \rightarrow f$  ("converges to").

The main reason we introduce the class of function  $\mathcal{S}(\mathbb{R})$  is that we now want to see the class of square-integrable functions  $L^2(\mathbb{R})$  (which will represent the physical wave function in following discussion) as linear functional over the space  $\mathcal{S}(\mathbb{R})$ . This will allow us to introduce a concept of derivative also in the case that  $f \in L^2(\mathbb{R})$  is not differentiable. Hence we define

**1.2.2 Definition (Temperate distributions).** Let be  $u : \mathcal{S}(\mathbb{R}) \rightarrow \mathbb{C}$  a functional. We call  $u$  a *temperate distribution* if it is continuous in  $\mathcal{S}(\mathbb{R})$ , in the sense that for every sequence  $\{f_n\} \in \mathcal{S}(\mathbb{R})$  which converges to a certain  $f \in \mathcal{S}(\mathbb{R})$ , we also have  $\lim_{n \rightarrow \infty} u(f_n) = u(f)$ . We indicate this set with the symbol  $\mathcal{S}'(\mathbb{R})$ .

Furthermore, for each  $u \in \mathcal{S}'(\mathbb{R})$  we define the derivative of  $u$  a distribution  $\partial_x^\alpha u \in \mathcal{S}'(\mathbb{R})$  such that

$$\partial_x^\alpha u(f) = (-1)^\alpha u(\partial_x^\alpha f) \quad \forall \alpha \in \mathbb{N}, \quad \forall f \in \mathcal{S}(\mathbb{R}). \quad (1.11)$$

We also define the multiplication of a temperate distribution  $u \in \mathcal{S}'(\mathbb{R})$  with a smooth function  $\varphi \in C^\infty(\mathbb{R})$ , the temperate distribution  $\varphi u$  defined as

$$\varphi u(f) := u(\varphi f) \quad \forall f \in \mathcal{S}(\mathbb{R}). \quad (1.12)$$

Now we have the following proposition

**1.2.3 Proposition.** Take the Hilbert space  $L^2(\mathbb{R})$ . Then, we have  $L^2(\mathbb{R}) \hookrightarrow \mathcal{S}'(\mathbb{R})$ . This means that for every  $g \in L^2(\mathbb{R})$  the functional defined in  $\mathcal{S}(\mathbb{R})$  as

$$(g|f) = \int_{-\infty}^{+\infty} \overline{g(x)} f(x) dx, \quad \text{with } f \in \mathcal{S}(\mathbb{R}) \quad (1.13)$$

is a temperate distribution.

The last proposition means that every square-integrable function can be thought as a continuous functional in this Schwartz space and that we can always thought all those functions as differentiable (in the sense of distributions).

After this preamble we could finally define the Fourier transform.

**1.2.4 Definition (Fourier transform).** Let be  $f \in \mathcal{S}(\mathbb{R})$ . We call the Fourier transform of  $f$  the function defined as follow:

$$\widehat{f}(p) \equiv \mathcal{F}[f](p) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-ipx} f(x) dx. \quad (1.14)$$

Moreover, we define the Fourier Transform of a temperate distribution  $u \in \mathcal{S}'(\mathbb{R})$  a functional  $\widehat{u}$  defined as follow:

$$\widehat{u}(f) \equiv \mathcal{F}[u](f) = u(\widehat{f}) \quad \forall f \in \mathcal{S}(\mathbb{R}). \quad (1.15)$$

It could be proved (see [2, Chap. 8]) that for each  $f \in \mathcal{S}(\mathbb{R})$  and  $u \in \mathcal{S}'(\mathbb{R})$ , their Fourier transform also lies respectively on  $\mathcal{S}(\mathbb{R})$  and  $\mathcal{S}'(\mathbb{R})$  and that there exist the inverse transformation  $\mathcal{F}^{-1}$  defined as

$$\mathcal{F}^{-1}[g](x) \equiv \check{g}(x) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ipx} g(p) dp \quad \text{with } g \in \mathcal{S}(\mathbb{R}), \quad (1.16)$$

$$\mathcal{F}^{-1}[u](f) \equiv \check{u}(f) := u(\check{f}) \quad \text{with } u \in \mathcal{S}'(\mathbb{R}), \quad \forall f \in \mathcal{S}(\mathbb{R}), \quad (1.17)$$

Such that  $\mathcal{F}\mathcal{F}^{-1} = \mathbb{I}$ .

Once we defined the transformation  $\mathcal{F}$  we could report one of its most important properties, which is to transform derivatives in "position" space into multiplications in the "frequencies" space. Hence we enunciate this theorem.

**1.2.5 Theorem.** Let  $f \in \mathcal{S}(\mathbb{R})$ . Then, we have:

$$(a) \quad \widehat{x^\alpha f}(p) = (-i)^\alpha \partial_p^\alpha \widehat{f}(p) \quad \forall \alpha \in \mathbb{N}.$$

$$(b) \quad \widehat{\partial_x^\alpha f}(p) = (-i)^\alpha p^\alpha \widehat{f}(p) \quad \forall \alpha \in \mathbb{N}.$$

Now let  $u \in \mathcal{S}'(\mathbb{R})$ . Then, we have

$$(c) \quad \widehat{x^\alpha u} = (-i)^\alpha \partial_p^\alpha \widehat{u} \quad \forall \alpha \in \mathbb{N}.$$

$$(d) \quad \widehat{\partial_x^\alpha u} = (-i)^\alpha p^\alpha \widehat{u} \quad \forall \alpha \in \mathbb{N}.$$

*Proof.* For point (a), we only need to re-write the function inside the integral (1.14)  $e^{ipx} x^\alpha f(x)$  as  $(-i)^\alpha \partial_p^\alpha e^{-ipx} f(x)$  and take the derivative outside the integral. In order to proving point (b), we must use integration by parts and transfer the derivation on  $f$  into a derivation on  $e^{-ipx}$ . So we can obtain our hypotesis. Point (c) and (d) can be proved by considering the distributions  $\widehat{x^\alpha u}$  and  $\widehat{\partial_x^\alpha u}$  acting on some test function  $f \in \mathcal{S}(\mathbb{R})$ , and then using the definitions 1.2.2, 1.2.4 and points (a), (b) to verify our thesis. ■

At this point of the section we are interested on thinking about the set  $L^2(\mathbb{R})$  as true functions and giving sense to equation (1.14) for those set, too. For this purpose, we enunciate the Plancherel's Theorem satisfying all our requests.

**1.2.6 Theorem (Plancherel's Theorem).** If  $u \in L^2(\mathbb{R})$ , then its  $\mathcal{S}'$ -Fourier transform  $\widehat{u}$  is also an element of  $L^2(\mathbb{R})$ , and their  $L^2$ -norms are identical

$$\|u\|_{L^2} = \|\widehat{u}\|_{L^2}. \quad (1.18)$$

Then the Fourier transform could be thought as a linear isometric operator in the Hilbert space  $L^2(\mathbb{R})$ .

The proof of this Theorem could be also found in [2, Chap. 9]. Finally, we managed to give a rigorous definition of Fourier transform for square-integrable functions.

The next argument that we must introduce about Fourier transformation in the concept of convolution product. Hence we define:

**1.2.7 Definition (Convolution product).** Let be  $f, g \in L^2(\mathbb{R})$ . We define the convolution product of  $f$  and  $g$  the function defined as

$$f \star g(x) := \int_{-\infty}^{+\infty} f(x-y)g(y) dy \quad (1.19)$$

Once we defined the convolution product, we need to enunciate a theorem that will be useful during the investigation of our thesis.

**1.2.8 Theorem (Convolution theorem).** For all  $v, u \in L^2(\mathbb{R})$ , the following identities holds:

- (i)  $\widehat{u \star v} = \widehat{u}\widehat{v}$ ,
- (ii)  $\widehat{uv} = (2\pi)^{-\frac{1}{2}}\widehat{u} \star \widehat{v}$

Now we can pass to the final section this first chapter and discuss about the basic concepts of quantum mechanics.

### 1.3 Quantum Mechanics

In the last part of this chapter we are going to investigate the foundations of quantum mechanics. The crucial points about the behavior of quantum systems could be outlined as follow (a deeper investigation on quantum basic axioms has done by W. Moretti in [1, Chap. 7]):

- (A1) The result of a measure on a quantum system with fixed state has only probabilistic outcome. It is not possible to known the exact result of a measure (i.e. the position of a particle), but only the probability of each possible result. However, if a physical quantity has been measured, a second measure done immediately after the first one, will give the same result.
- (A2) There exist *non-compatible* physical quantities. In the sense that when we make a measure of the quantity  $A$  and obtain the value  $a_1$ , and immediately after we make a measure of its incompatible quantity  $B$  and obtain the value  $b$ , If we immediately repeat the measure of  $A$ , this will give a value  $a_2 \neq a_1$  in general. Furthermore, it's been seen that incompatible quantities are never functions one of the other and there not exist experimental apparatus able to measure at the same time the two quantities.

There also exist *compatible* quantities in the following sense. Suppose that  $A'$  and  $B'$  are physical quantities of this type, then we make two successive and arbitrarily close measures of  $A'$  and  $B'$ , obtaining the values  $a$  and  $b$  respectively. If we make a third measure arbitrarily close to the other two of the quantity  $A'$ , we will obtain again the value  $a$ . And the same happens if we exchange  $A'$  with  $B'$ . It's has been seen that each quantity  $A$  is self-compatible and that if a quantity  $B$  is function of another quantity  $C$ , then they are compatible.

In Quantum Mechanics the quantities which are measurable on physical system and whose behavior is described by (A1) and (A2) are called *observable*. In classical mechanics, observables are described as "smooth" functions defined on the phase space of generalized coordinates  $(q_i, p_i)$ .



Instead in quantum mechanics, observables are thought as Hermitian operators defined in some Hilbert space and the physical state of our quantum system is thought as a vector living in this space with norm. Hence, we have the following statements:

- (A3) Observable are associated to Hermitian operators  $A : D(A) \rightarrow \mathcal{H}$  defined in some Hilbert space  $\mathcal{H}$  and the all the possible results of a measurement are given by the spectrum  $\sigma(A)$ .
- (A4) The physical state of a quantum system is associated with a vector  $\psi$  on this Hilbert space  $\mathcal{H}$ . This vector gives us all the information required to define the distribution probability of all the possible outcome. In fact, the probability of measuring a certain value or set of values  $P_{\Delta}^{(A)}$  (probability that a measure of  $A$  gives a number inside the set  $\Delta \subseteq \mathbb{R}$ ) is given by the following equation:

$$P_{\Delta}^{(A)} := (\psi | P \psi), \quad (1.20)$$

where  $P$  is a projector operator in the eigenspace associated with the elements of  $\sigma(A)$  inside  $\Delta$ . Furthermore, the expectation value  $\langle A \rangle$  of such observable  $A$  is given by

$$\langle A \rangle = (\psi | A \psi). \quad (1.21)$$

In addition, the projector associated to all the real set  $\mathbb{R}$  has to be the identity  $\mathbb{I}$  because the proposition "the result of a measure it's a real number" it's always real. Then, it must be

$$P_{\mathbb{R}}^{(A)} = (\psi | \psi) = 1, \quad (1.22)$$

which implies  $\|\psi\| = 1$ .

From the last equation we can understand why the observable  $A$  has to be Hermitian. Since the result of our measures are real numbers, we want  $A$  to have  $\langle A \rangle \in \mathbb{R}$  and  $\sigma(A) \subseteq \mathbb{R}$ , but these conditions are implied by the fact that  $A$  is Hermitian.

**1.3.1 Example.** Let's consider the "position" operator defined in the first part of the chapter. It is an operator  $X : D(X) \rightarrow L^2(\mathbb{R})$  with  $D(X)$  is a dense subspace of  $L^2(\mathbb{R})$  (i.e.  $D(X) = C_0^\infty(\mathbb{R})$ ), which maps  $f \mapsto xf$ . It is called the "position" operator because it is really the Hermitian (also symmetric) operator associated with the measure of the position of a particle. A particle instead is described by a function  $\psi \in L^2(\mathbb{R})$  (also called "wave function") such that

$$\|\psi\|_{L^2}^2 = \int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1. \quad (1.23)$$

Here  $|\psi(x)|^2$ , following statement (A4), has the value of density probability function for the position of our particle. Moreover, the projector operator associated with a certain interval  $(a, b) \subset \mathbb{R}$  is the characteristic function  $\chi_{(a,b)}$  (the function which is zero outside  $(a, b)$  and one inside) and the probability of finding the particle inside  $(a, b)$  is given by:

$$P_{\Delta}^{(X)} = (\psi | \chi_{(a,b)} \psi) = \int_{-\infty}^{+\infty} \chi_{(a,b)}(x) |\psi(x)|^2 dx = \int_a^b |\psi(x)|^2 dx. \quad (1.24)$$

Instead the expectation value of  $X$  is given by:

$$\langle X \rangle = (\psi | X \psi) = \int_{-\infty}^{+\infty} x |\psi(x)|^2 dx. \quad (1.25)$$

**1.3.2 Example.** Another example is the "momentum" operator  $P := -i\partial_x$ . In this case,  $P$  represents the Hermitian (symmetric) operator associated to the physical quantity of momentum and it's defined in the same Hilbert space of  $X$ . Note that if we take the Fourier transform of a wave function  $\psi \in L^2(\mathbb{R})$  we have

$$P\psi = P\mathcal{F}^{-1}\mathcal{F}\psi = \frac{-i}{\sqrt{2\pi}}\partial_x \int_{-\infty}^{+\infty} e^{ipx} \widehat{\psi}(p) dp = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ipx} p \widehat{\psi}(p) dp, \quad (1.26)$$

Which means that the operator  $P$  has a double face: it acts as a derivative operator in one space (which could be called the "position" space), but as a multiplicative operator in the transformed space (called the "momentum" space). The same thing could be said in the opposite way for the operator  $X$ .

**1.3.3 Remark.** Considering particles of mass  $m > 0$ , it will be convenient to work with dimensionless variables  $x$ ,  $p$ , etc., and dimensionless functions by using a length scale  $\ell$  as the unit of length,  $\hbar/\ell$  as the unit of momentum,  $m\ell^2/\hbar$  as the unit of time, and  $\hbar^2/m\ell^2$  as the unit of energy, effectively setting  $m = \hbar = 1$ .

Once we defined this first fundamental statements about quantum mechanics, we focus on the time evolution of a physical system. We are interested in the equation which determines how the vector  $\psi$  which describe our system evolves in the Hilbert space when the system (our particle) is under the action of some external force (a energy potential). This role, in non-relativistic quantum mechanics, is played by *Schrödinger equation*. Hence we have

(A5) The time evolution of a physical state, described by a vector  $\psi$  in some Hilbert space  $\mathcal{H}$  is given by the *Schrödinger equation*

$$i\partial_t\psi = H\psi \quad (1.27)$$

where  $H$  is the Hamiltonian Hermitian operator and represents the operator associated with the energy of a physical system and we can write its expectation value as

$$\langle H \rangle = (\psi|H\psi). \quad (1.28)$$

In the case of particles which travels in the physical space and subjected to some potential  $V(x)$  and described by the Hilbert space  $L^2(\mathbb{R})$  (the case of our interest), the Hamiltonian  $H$  could is given by the following

$$H := \frac{1}{2}P^2 + V(X) \quad (1.29)$$

where  $P^2/2$  is called the "kinetic energy" operator and  $V(X)$  is the operator which maps  $\psi \mapsto V(X)\psi := V(x)\psi(x)$ . Here  $H$  it could be brought back to the classical mechanical energy of a particle which travels across a potential  $V$  (remember that here we have set the mass of our particles  $m = 1$ ).

Now we want to find a general solution for this equation. In particular, given a fixed initial state  $\psi(0)$  for our physical system, we want to determine the final state at a certain time  $\psi(t)$ . In order to find these solutions, we must define the exponential operator

**1.3.4 Definition.** Let  $A \in \mathcal{B}(\mathcal{H})$  where  $\mathcal{H}$  is an Hilbert space. Then we define the operator  $\exp(A)$  as

$$\exp(A) := \sum_{n=0}^{\infty} \frac{A^n}{n!} \quad (1.30)$$

**1.3.5 Observation.** The sum reported in the previous definition must be read in this way: the sequence of partial sums  $S_m := \sum_{n=0}^m A^n/n!$  converges to some operator in the space  $\mathcal{B}(\mathcal{H})$ , in the sense that there exists an operator  $\exp(A) \in \mathcal{B}(\mathcal{H})$  such that  $\lim_{m \rightarrow \infty} \|S_m - \exp(A)\| = 0$ .

Once we defined the map  $\exp$  for bounded operators, we can give a general formula for the solutions of Schrödinger equation. In fact, given a certain Hamiltonian  $H$  for our system, let's consider the operator

$$U(t) := \exp(-iHt) = \sum_{n=0}^{\infty} \frac{(iHt)^n}{n!} \quad (1.31)$$

and suppose that this sum is well-defined.  $U(T)$  is called *unitary evolution operator* and it tells us how a fixed initial state evolve with time. In fact, if we take a vector  $\psi_0 \in \mathcal{H}$  with  $\|\psi_0\| = 1$  as initial state, then the vector  $\psi_t := U(t)\psi_0$  is the solution of our Schrödinger equation since

$$i\partial_t \psi_t = i\partial_t \exp(-iHt)\psi_0 = i(-iH)\exp(-iHt)\psi_0 = H\psi_t. \quad (1.32)$$

It could be seen that  $U(t)$  is Hermitian and that  $U(t)^*U(t) = \mathbb{I}$  (from here the term *unitary*) so that it doesn't change the normalization of our vector:

$$\|\psi_t\|^2 = (U(t)\psi_0|U(t)\psi_0) = (\psi_0|U(t)^*U(t)\psi_0) = \|\psi_0\|^2 = 1. \quad (1.33)$$

At this level, it's useful to introduce the concept of *density probability current*.

**1.3.6 Definition.** Let be  $\psi \in L^2(\mathbb{R})$  a function. Then the density probability current is the function defined by

$$j_\psi(x, t) := \frac{1}{2i} [\partial_x \psi(x, t) \psi^*(x, t) - \psi(x, t) \partial_x \psi^*(x, t)], \quad (1.34)$$

This quantity gives us information about probability flows in the space and its bounded with the density probability function  $\rho(x, t) := |\psi(x, t)|^2$  by the *continuity equation*

$$\partial_t \rho(x, t) + \partial_x j_\psi(x, t) = 0. \quad (1.35)$$

Now, we turn back to our physical particles described by square-integrable functions and consider the Hamiltonian  $H_0$  given by only the kinetic term of equation (1.29)  $H_0 = P^2/2$ . This Hamiltonian represents the evolution of free particles which are not subjected by any external potential. We note that in this case, solutions given by  $U(t)\psi_0 = \exp(-iH_0t)\psi_0$  have a simple form. Since the derivative operator  $P$  could be seen as a multiplicative operator in the Fourier-transformed space, then the exponential operator  $\exp(-iP^2t/2)$  could be seen as a multiplicative phase in the "momentum" space.

$$\exp(-iP^2t/2) \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ipx} \widehat{\psi_0}(p) dp = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ip(x-pt/2)} \widehat{\psi_0}(p) dp \quad (1.36)$$

In presence of a generic potential  $V(x)$ , things are more complicated. In these case it's helpful to introduce the *interaction picture*. In this picture we consider the wave function of our particle at some time  $\psi_t$  not as the evolution from an initial state  $\psi_0$  under unitary operator  $U(t)$ . The reasoning here is the following: consider firstly a wave function  $\psi$  at some time. Then let it evolve backwards in time under the free Hamiltonian  $H_0 = P^2/2$ . After that, turn forward the time arrow and make everything evolve to the initial time under the unitary operator defined by the complete Hamiltonian  $H = H_0 + V(X)$ . Now  $\psi$  has no more the value of the initial state of our particle, but the state that this particle would have had without the potential  $V$ , while this two time evolutions gives us the "interacted" wave function at some time. This picture could be described by introducing the *Møller operator*  $\Omega_V$ .

**1.3.7 Definition.** Let  $H_0 = P^2/2$  the free Hamiltonian and  $H = P^2/2 + V(X)$  an interacting Hamiltonian for some potential  $V$ . We define the **Møller operator**  $\Omega_V$  as follow:

$$\Omega_V := \lim_{t \rightarrow -\infty} e^{iHt} e^{-iH_0 t} \quad (1.37)$$

This considerations will be useful in the last part of our thesis.  
 Now we introduced all the mathematical tools necessary to deal with all the contents of our thesis and we are ready to start our relation about *quantum backflow*.

## Chapter 2

# Quantum Backflow - Basic Concepts

In this chapter we start our discussion on backflow effect. First of all, we will give some historical introduction about first observations and subsequently deeper analysis. Then, we will give a rigorous definition of backflow reporting some illustrative and relevant examples. In the central part of this chapter we will focus about outlining the basic properties of backflow in free theories (with particles which evolves under the free Hamiltonian  $H_0 = P^2/2$ ). For this purpose, we will retrace the first work of Braken and Melloy [4] written in 1994, outlining its most important results and discussing in detail and rigorously their dissertation.

As we remarked in Section 1.3, considering particles of mass  $m > 0$ , it will be convenient to work with dimensionless variables for position  $x$ , momentum  $p$ , etc., and dimensionless functions (such as the wave function  $\psi$  and the current  $j_\psi$ ) by using a length scale  $\ell$  as the unit of length,  $\hbar/\ell$  as the unit of momentum,  $m\ell^2/\hbar$  as the unit of time, and  $\hbar^2/m\ell^2$  as the unit of energy, effectively setting  $m = \hbar = 1$ .

### 2.1 Historical Introduction

Let's start by contextualizing the problem from which quantum backflow arises. Take a particle bounded to travel on a straight line (currently suppose the particle to be free from any kind of potential). As we said in the introductory section about Quantum Mechanics, all particles are described by a wave function  $\psi(x, t)$  whose square absolute value  $|\psi(x, t)|^2$  gives the probability density of finding the particle in some point of space  $x$  at some time  $t$ . On the other hand, if we take the Fourier transform of our wave function  $\hat{\psi}(p, t)$ , its square absolute value  $|\hat{\psi}(p, t)|^2$  gives the density probability of finding the particle with a certain "momentum" (i.e. velocity)  $p$ .

Now suppose to shot this quantum particle with a defined positive velocity along our straight line, in the sense that  $\hat{\psi}(p) \neq 0$  only for  $p > 0$ . Now consider the probability  $P(t)$  of finding the particle behind a certain point (take the origin  $x = 0$ ) at some time  $t$ . This quantity is given by

$$P(t) := \int_{-\infty}^0 |\psi(x, t)|^2 dx \quad (2.1)$$

Now we bring the following question:

*For each wave function with strictly positive momentum, is the quantity  $P(t)$  always decreasing with time? Or it could increase in certain cases?*

Classically, the answer is obvious. If you take a particle with positive velocity, its position certainly increases with time. Instead in Quantum Mechanics, things are more exotic and wave functions with positive velocity, but increasing  $P(t)$  exist. This is *quantum backflow*.

First observations about this phenomenon date back to 1969 in a work written by Allcock [3] about the problem of time arrival as a physical observable in quantum mechanics. After that, backflow has been neglected until 1994, when Bracken and Melloy made an exhaustive investigation outlining the fundamental properties and quantitative bounds in free theory (no potential on the particles). Subsequently, Eveson, Fewster and Verch [6] described backflow as a fundamental quantum inequality and in 2013 Palmero [7] gave suggestion for experimental observation using Bose-Einstein condensate. The analysis of the results obtained by Bracken and Melloy will be discussed in this chapter while the next one will discuss mainly the study of backflow in scattering theory (particles subjected to a potential) treated in the recent work of Bostelmann, Cadamuro and Lechner [5]. Now we continue our discussion giving a complete mathematical model and examples of backflow.

## 2.2 Definition of Backflow and Illustrative Examples

The first goal of this section is to give complete set of definitions in order to clarify the nature of backflow and the mathematics the lies behind it. We start by clarifying what we mean by particles with only positive momentum introducing the concept of *right-movers*.

**2.2.1 Definition (Right-mover).** Let  $\psi \in L^2(\mathbb{R})$  a wave-function associated to a physical quantum particle and  $|\psi(x)|^2$  the density probability of position measuring.  $\psi$  is called a *right-mover* if  $\text{supp } \hat{\psi} \in [0, +\infty)$ .

It could be seen that the set of all right-movers is a closed subspace of the Hilbert space  $L^2(\mathbb{R})$ . Then, will turn useful to define a projector operator which transform each kind of wave-function into a right-mover.

**2.2.2 Definition.** We define the operator  $E_{\pm} : L^2(\mathbb{R}) \rightarrow L^2(\mathbb{R})$  as:

$$\mathcal{F}[E_{\pm}\psi](p) = \vartheta(\pm p)\hat{\psi}(p) \quad \forall \psi \in L^2(\mathbb{R}), \quad (2.2)$$

where  $\vartheta$  is the Heaviside function defined as:

$$\vartheta(p) = \begin{cases} 0 & p \leq 0 \\ 1 & p > 0 \end{cases}. \quad (2.3)$$

This operator does no more than taking the representation of the wave-function in momentum space and "cut-off" all the negative (positive in case of  $E_-$ ) velocities. We can prove that this operator is a real projector in the sense of the definition 1.1.17.

**2.2.3 Proposition.** Let  $E_+$  be the operator of definition 2.2.2. Then,  $E_+$  is bounded, self-adjoint and  $E_+^2 = E_+$ .

*Proof.* The boundedness is a consequence of Plancherel's Theorem. In fact, for all  $\psi \in L^2(\mathbb{R})$  with  $\|\psi\| = 1$

$$\|E_+\psi\| = \|\mathcal{F}[E_+\psi]\| = \|\vartheta\hat{\psi}\| \leq \|\hat{\psi}\| = \|\psi\| = 1 \quad (2.4)$$

Self-adjointness is given by the unity of Fourier transform

$$(\psi|E_+\phi) = (\hat{\psi}|\widehat{E_+\phi}) = (\hat{\psi}|\vartheta\hat{\phi}) = (\vartheta\hat{\psi}|\hat{\phi}) = (E_+\psi|\phi) \quad \forall \phi, \psi \in L^2(\mathbb{R}), \quad (2.5)$$

while  $E_+^2 = E_+$  is given by the definition. ■

Note that from this definition we can re-define equivalently every right-mover as those wave-functions  $\psi$  such that  $E_+\psi = \psi$ . Henceforth, we will write the set of all right-movers with the symbol  $E_+(L^2)$ .

Once we have introduced these concepts, we are able to give an exhaustive definition of backflow. Hence, we give the following statement:

*Given a right-mover  $\psi = E_+\psi$ , backflow occurs whenever the density probability current function  $j_\psi = -i/2[\psi^*\partial_x\psi - \psi\partial_x\psi^*]$  assumes negative values.*

Now we are interested to show clearly that backflow is a truly quantum effect predicted by the non-relativistic mono-dimensional Schrödinger equation. In order to pursue this aim, we will illustrate some examples in which backflow occurs.

### 2.2.1 Superposition of Plane Waves

The first instructive example is given by the function of the form:

$$\begin{aligned} \psi(x, t) &= Ae^{i\vartheta_1(x, t)} + Be^{i\vartheta_2(x, t)}, \\ \text{where } \vartheta_n(x, t) &= \left[ p_n \left( x - \frac{p_n t}{2} \right) + \gamma_n \right] \quad n = 1, 2. \end{aligned} \quad (2.6)$$

Here we choose  $A, B, p_1$  and  $p_2$  positive constant, while  $\gamma_1$  and  $\gamma_2$  are arbitrary real numbers. We did nothing more than take the sum of two plane waves (which are eigenfunction of the free-particle Hamiltonian) with positive momentum  $p_n$  and energy  $p_n^2/2$  for  $n = 1, 2$ . This obviously does not represent a real state because it's not normalizable, nevertheless it could be really interesting studying how backflow could emerge from such a simple case. In fact, now we can evaluate the density probability current  $j_\psi(x, t)$  in a certain point  $x \in \mathbb{R}$  at the instant  $t \in \mathbb{R}$ . Remembering the definition of  $j_\psi(x, t)$  we quickly obtain:

$$j_\psi(x, t) = A^2 p_1 + B^2 p_2 + AB(p_1 + p_2) \cos(\vartheta_1(x, t) - \vartheta_2(x, t)). \quad (2.7)$$

We can easily check that  $\vartheta_1(x, t) - \vartheta_2(x, t)$  is linearly dependent with the time  $t$ , so easy to understand that the density current could vary from an upper value of  $(p_1 A + p_2 B)(A + B)$  to a lower value of  $(p_1 A - p_2 B)(A - B)$ . If, for example  $A > B$  and  $p_1 A < p_2 B$ , this lower value is negative and so backflow occurs.

Although this example has not a physical interpretation, because of the non-normalizability of plane waves, we can note that backflow is essentially an interference effect between of some wave-packets with high positive momentum and others with low positive momentum. This aspect is not banal and we will re-use it for proving an important theorem regarding the intensity of backflow through a single point at a some instant of time. In particular, we will construct a normalized wave-packet in the momentum space as a sum of a function  $\tilde{\chi}(p) \in L^2(\mathbb{R}_+)$  and his translation  $\tilde{\chi}(p - n)$  and this coincides with taking the interference of two wave-packets with different positive momenta.

### 2.2.2 Superposition of Gaussian Wave-packets

Another example can be made by replacing the two plane waves with Gaussian tightly picked in momentum. This represent a more physically realistic state. We consider the sum of two initial Gaussian wave-packets with equal spatial width  $\sigma$ , evolved for a time  $t$ . The corresponding normalized wave function is

$$\psi(x, t) = \sum_{n=1,2} C_n \frac{1}{\sqrt{4\sigma^2 + 2it}} \exp \left( ip_n(x - p_n t) - \frac{(x - p_n t)^2}{4\sigma^2 + 2it} \right), \quad C_n \in \mathbb{R}, \quad p_1, p_2 > 0. \quad (2.8)$$

This function was given by Yearsley in [8]. As in the previous example, this wave-function is given by the superposition of two waves with different momentum. Note that for  $\sigma \rightarrow 0$ , we obtain again the superposition of plane waves above. To prove that for such a function backflow occurs, we set the parameters  $p_1, p_2, C_1, C_2$  and  $\sigma$  to be

$$p_1 = 0.3, p_2 = 1.4, C_1 = 1.8, C_2 = 1, \sigma = 10. \quad (2.9)$$

and plot the probability  $P(t)$  of remaining in  $x < 0$  as a function of time. This plot is shown in Figure [2.2]. we can see that  $P(t)$  is not monotonically decreasing, but in several disjoint time intervals it increases, proving the presence of backflow.

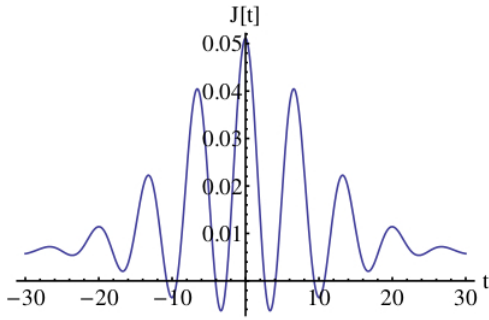


FIGURE 2.1: Plot of the current for a superposition of two gaussians, with the parameters given in Eq. [2.9].

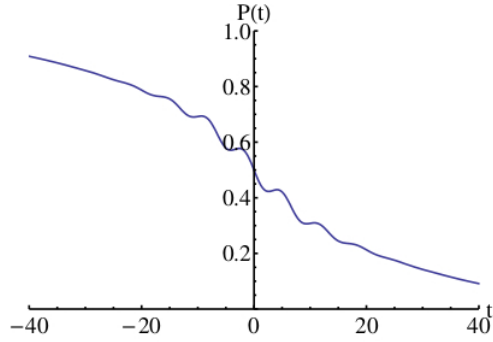


FIGURE 2.2: Plot of the probability for remaining in  $x < 0$  for a superposition of two gaussians, with the parameters given in Eq. [2.9].

The question is now; how much probability backflow does this state display? To answer this question, we need the probability flux by evaluating

$$P(t_1) - P(t_2) = \int_{t_1}^{t_2} j_\psi(0, t) dt, \quad (2.10)$$

Where  $P$  is the probability of finding the particle in  $x < 0$  and  $[t_1, t_2]$  the interval during which gives the largest amount of backflow for this wave-function. Calculations show that,

$$F := \inf\{P(t_1) - P(t_2) \mid t_2 > t_1\} \approx -0.0061 \quad (2.11)$$

We will see in the following discussion that this approximately the 16% of the maximum amount of backflow theoretically allowed.

### 2.2.3 Normalizable Wave

The following example show that backflow can occur for normalizable wave-function, too. Let us consider a function  $\phi \in L^2(\mathbb{R})$  whose representation in the momentum space (which is nothing more than its Fourier transform  $\hat{\phi}$ ) is given by the following equation:

$$\hat{\phi}(p) = \begin{cases} \frac{18}{\sqrt{35}K} p(e^{-p/K} - \frac{1}{6}e^{-p/2K}) & p > 0 \\ 0 & p \leq 0 \end{cases} \quad (2.12)$$

where  $K$  is a positive constant. This clearly represents a possible initial state for a physical particle. Now we can obtain the expression for the function  $\phi$  defined in the position space simply



by using Fourier anti-transform. In particular, after some calculation, we obtain:

$$\phi(x) = 18\sqrt{\frac{K}{70\pi}} \left[ \frac{1}{(1 - iKx)^2} - \frac{2}{3(1 - 2iKx)^2} \right]. \quad (2.13)$$

At this point we can quickly evaluate  $\phi(0)$ ,  $\phi'(0)$  and the density probability current  $j_\phi(0)$ :

$$\begin{aligned} \phi(0) &= 6\sqrt{\frac{K}{70\pi}} & \phi'(0) &= -12i\sqrt{\frac{K}{70\pi}} \\ j_\phi(0) &= -\frac{36K^2}{35\pi} < 0, \end{aligned} \quad (2.14)$$

which proves the presence of backflow. Evaluating the time evolution of this wave-function, the current is negative during the time interval  $[0, t_1]$  where  $t_1 \approx 0.021/K^2$ . The corresponding flux Eq.(2.10) for this period of backflow is

$$F \approx -0.0043 \quad (2.15)$$

## 2.3 Backflow in Free Theory

In this section we want to study the duration and the strength of this effect in the case of free particles. In particular, The question we ask ourself is the following:

*What is the maximum amount of probability which could flow back through a point  $x_0$  during an interval of time  $T$  for a right-moving free-particle?*

We will show that this problem is equivalent to the research of the smallest eigenvalue of a certain integral operator, and then we will evaluate an important bound for quantum backflow.

In the following discussion we will interpret the flux of probability defined in Eq. (2.10) in a time interval  $[0, T]$  through a certain point (the origin  $x = 0$ ) as the scalar product of the type  $(\hat{\psi}|\vartheta B_T \vartheta \hat{\psi})$ , where  $\hat{\psi}$  is the Fourier transform of our wave-function (i.e. right-mover),  $\vartheta$  is the Heaviside function (thought as a projector operator) and  $B_T$  is the *backflow operator* that will be proved to be bounded and self-adjoint. After that, we will link the search of upper bound for this operator to the search of the maximum eigenvalue of an integral operator  $K$  (defined by Bracken and Melloy in [4]). Furthermore, we will show that this maximum eigenvalue corresponds to the maximum amount of backflow allowed for any right-mover. In this part of our thesis will report the results obtained by Penz *et al.* in [10].

### 2.3.1 Temporal Boundedness of Backflow

Let's start by considering how the free Schrödinger evolution operator acts in the momentum space. We have seen in first chapter 1.3 that for a wave-function represented in the Fourier-transformed space  $\hat{\psi}$ , the evolution operator  $U_t$  acts as a phase multiplicative operator:

$$\hat{\psi}_t(p) := (U_t \hat{\psi})(p) = e^{-ip^2/2} \hat{\psi}(p). \quad (2.16)$$

Note that  $U_t^* = U_{-t}$ . The representation of such wave-functions in the "position" space are given by the anti-Fourier transform:

$$\psi_t(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ipx} \hat{\psi}_t(p) dp. \quad (2.17)$$

Let a particle have momentum space wave-function  $\widehat{\psi}$  at time 0. If  $\|\widehat{\psi}\| = 1$ , the probability that a position measurement at time  $t$  yields a position  $x > 0$  reads

$$L(\psi_t) := \int_0^{+\infty} |\psi_t(x)|^2 dx = (\widehat{\psi} | U_t^* \mathcal{F} \vartheta \mathcal{F}^{-1} U_t \widehat{\psi}). \quad (2.18)$$

Now we restrict to consider right-moving wave-functions  $\psi$  such that  $E_+ \psi = \psi$  or equivalently  $\vartheta \widehat{\psi} = \widehat{\psi}$  (i.e.  $\text{supp } \widehat{\psi} \subset \mathbb{R}_+$ ) and  $\|\psi\| = 1$ . Note that for such functions the evolution  $\psi_t$  is also a right-mover,  $\psi_t = E_+ \psi_t$ .

As shown in the previous examples, there exists some right-moving wave-functions in which backflow occurs and the probability  $L(\psi_t)$  does decrease in some interval. So is convenient to define the maximum backflow for a fixed right-mover  $\psi$  as

$$\lambda(\psi) = \{L(\psi_s) - L(\psi_t) \mid \psi = E_+ \psi, \|\psi\| = 1, t > s\} \quad (2.19)$$

But we are interested in the maximum amount of probability backflow. So, we define the *backflow constant*  $\lambda$  as

$$\lambda := \sup\{\lambda(\psi) \mid \psi = E_+ \psi, \|\psi\| = 1\}. \quad (2.20)$$

Introducing the orthogonal projector  $\tilde{\vartheta}_t := U_t^* \mathcal{F} \vartheta \mathcal{F}^{-1} U_t$  we obtain for any normalized wave-function  $\psi \in L^2(\mathbb{R})$

$$L(\psi_s) - L(\psi_t) = (\widehat{\psi} | (\tilde{\vartheta}_s - \tilde{\vartheta}_t) \widehat{\psi}). \quad (2.21)$$

Now, because of

$$\tilde{\vartheta}_s - \tilde{\vartheta}_t = U_{\frac{t+s}{2}}^* (\tilde{\vartheta}_{\frac{s-t}{2}} - \tilde{\vartheta}_{\frac{t-s}{2}}) U_{\frac{t+s}{2}}, \quad (2.22)$$

we can write

$$\lambda = \sup\{(\widehat{\psi} | U_\tau^* (\tilde{\vartheta}_{-T} - \tilde{\vartheta}_T) U_\tau \widehat{\psi}) \mid \psi = E_+ \psi, \|\psi\| = 1, \tau \in \mathbb{R}, T > 0\}, \quad (2.23)$$

Now we define

**2.3.1 Definition.** Given a fixed time  $T > 0$ . We call the **backflow operator**  $B_T : L^2(\mathbb{R}) \rightarrow L^2(\mathbb{R})$  as

$$B_T := \tilde{\vartheta}_{-T} - \tilde{\vartheta}_T. \quad (2.24)$$

Once we defined  $B_T$  we have the following proposition

**2.3.2 Proposition.** The operator  $\vartheta B_T \vartheta$  with  $B_T$  defined in Eq. (2.24) is bounded and self-adjoint.

*Proof.* The boundedness of  $\vartheta B_T \vartheta$  follows from the boundedness of  $\vartheta$  and  $U_T$  for all  $T \in \mathbb{R}$ . One can prove self-adjointness by considering the scalar product  $(\psi | \vartheta B_T \vartheta \phi)$  for some  $\psi, \phi \in L^2(\mathbb{R})$  and see that it is equal to  $(\vartheta B_T \vartheta \psi | \phi)$  using self-adjointness of  $\vartheta$  and the definition of adjoint for  $U_T$ .  $\blacksquare$

Note that the operator  $\vartheta$  here needs to cut the negative velocities of a wave-function transforming it into a right-mover.

Turning back to analysis of backflow constant  $\lambda$ , since the unitary  $U_\tau$  stabilizes the set of right-movers  $E_+(L^2)$ , we have

$$\lambda = \sup\{(\phi | \vartheta B_T \vartheta \phi) \mid \phi \in L^2(\mathbb{R}), \|\phi\| = 1, T > 0\}, \quad (2.25)$$

or equivalently

$$\lambda = \sup \bigcup_{T>0} \sigma(\vartheta B_T \vartheta). \quad (2.26)$$

This equation could be simplified by neglecting the set sum over  $T > 0$ . In fact we see that  $\vartheta B_T \vartheta$  is the operator which gives us the flux of probability through the origin  $x = 0$  for a time interval  $[0, T]$ . But now we will use scaling arguments to see that backflow is independent to the time  $T$ , in the sense that for every right-mover who gives some amount of backflow during the interval  $[0, T]$ , then there exists another right-mover which gives the same backflow, but for a time interval  $[0, T']$  arbitrarily larger. Hence we have

**2.3.3 Proposition.** *For any fixed time  $T > 0$  holds  $\lambda = \sup \sigma(\vartheta B_T \vartheta)$ .*

*Proof.* Consider the family of unitary dilatation operators  $V_\mu : L^2(\mathbb{R}) \rightarrow L^2(\mathbb{R})$  with  $\mu > 0$  defined as  $(V_\mu \phi)(p) := \sqrt{\mu} \phi(\mu p)$ . we can see that for any  $\phi \in L^2(\mathbb{R})$

$$(\vartheta V_\mu \phi)(p) = \sqrt{\mu} \vartheta(p) \phi(\mu p) = \sqrt{\mu} \vartheta(\mu p) \phi(\mu p) = (V_\mu \vartheta \phi)(p), \quad (2.27)$$

and

$$\mathcal{F} \vartheta \mathcal{F}^{-1} V_\mu \phi = \mathcal{F} \vartheta V_{1/\mu} \mathcal{F}^{-1} \phi = \mathcal{F} V_{1/\mu} \vartheta \mathcal{F}^{-1} \phi = V_\mu \mathcal{F} \vartheta \mathcal{F}^{-1} \phi. \quad (2.28)$$

Then  $V_\mu$  commute with both the operator  $\vartheta$  and  $\mathcal{F} \vartheta \mathcal{F}^{-1}$ . Note that  $V_\mu^* = V_{1/\mu}$ . Now we see from a brief calculation that

$$V_\mu U_t V_\mu^* = U_{\mu^2 t} \quad (2.29)$$

From this it follows that

$$V_\mu \vartheta B_T \vartheta V_\mu^* = \vartheta B_{\mu^2 T} \vartheta. \quad (2.30)$$

Since the spectrum of an operator is invariant under a unitary transformation we have for any  $T_1, T_2 > 0$

$$\sigma(\vartheta B_{T_1} \vartheta) = \sigma(V_{\mu'} \vartheta B_{T_1} \vartheta V_{\mu'}^*) = \sigma(\vartheta B_{T_2} \vartheta) \quad \text{where } \mu' = \sqrt{T_2/T_1}. \quad (2.31)$$

Hence we can write  $\lambda = \sigma(\vartheta B_{T_1} \vartheta)$  for any fixed  $T > 0$ . ■

Summing up all the results we obtained for the backflow operator  $B_T$  and the backflow constant  $\lambda$ , we have arrived to one of the main goal of our dissertation.

**2.3.4 Theorem (Temporal Boundedness of Backflow).** *Let be  $\lambda$  the backflow constant defined by  $\lambda = \sup \sigma(\vartheta B \vartheta)$ , where  $B = B_{T=1}$  is the backflow operator. Then, for any right-mover  $\psi \in L^2(\mathbb{R})$  such that  $\psi = E_+ \psi$  and for any  $T > 0$  we have*

$$\int_0^T j_\psi(0, t) dt \geq -\lambda > -\infty. \quad (2.32)$$

*Proof.* The fact that  $\lambda$  is the maximum amount of backflow is given by definition (see the previous discussion). We just only to prove that  $\lambda$  is finite. But since the operator  $\vartheta B \vartheta$  is bounded and self-adjoint (from Prop. 2.3.2) we have

$$\sigma(\vartheta B \vartheta) \subseteq [-\|B\|, \|B\|]. \quad (2.33)$$

Hence we have our thesis. ■

Once we proved that backflow is time-bounded for free particles we are interested about evaluating numerically the backflow constant  $\lambda$  introducing the integral operator first founded by Bracken and Melloy. These authors heuristically introduce  $\lambda$  via time integrals of currents at point  $x = 0$  over arbitrary finite intervals. From this they motivate their final definition of  $\lambda$  as the supremum of the spectrum of the integral operator

definitio  
Now we will prove that this two definitions of  $\lambda$  are equivalently.

**2.3.5 Proposition.** Let  $K : L^2(\mathbb{R}_+) \rightarrow L^2(\mathbb{R}_+)$  the integral operator defined by:

$$(Kf)(u) = -\frac{1}{\pi} \int_0^\infty \frac{\sin(u^2 - v^2)}{u - v} f(v) dv \quad \forall f \in L^2(\mathbb{R}_+). \quad (2.34)$$

Then we have  $\vartheta B \vartheta f = Kf$  for any  $f \in L^2(\mathbb{R}_+)$ .

*Proof.* Since  $\vartheta B \vartheta$  is bounded we only need to prove  $\vartheta B \vartheta = K$  on a dense subspace of  $L^2(\mathbb{R}_+)$ . Hence, we choose  $\mathcal{S}(\mathbb{R}_+)$ , the space of all smooth functions, rapidly decreasing and with support contained in  $\mathbb{R}_+$ .

First of all, we demonstrate a relation between the orthogonal projection  $\mathcal{F} \vartheta \mathcal{F}^{-1}$  and the Hilbert transformation defined as

$$H : L^2(\mathbb{R}) \rightarrow L^2(\mathbb{R}), \quad (Hf)(p) = \frac{1}{\pi} PV \int_{-\infty}^\infty \frac{f(q)}{p - q} dq. \quad (2.35)$$

Here  $PV$  indicates that the improper integral is meant as the principal value. For  $f \in \mathcal{S}(\mathbb{R})$  we obtain by means of Lebesgue's dominated convergence theorem and by means of Sochozki's formula (see [11, Example 3.3.1])

$$\begin{aligned} (\mathcal{F} \vartheta \mathcal{F}^{-1} f)(p) &= \frac{1}{2\pi} \int_0^\infty e^{-ipx} \left( \int_{-\infty}^\infty e^{ixq} f(q) dq \right) dx \\ &= \frac{1}{2\pi} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^\infty f(q) \left( \int_0^\infty e^{i(q-p)x - \varepsilon x} dx \right) dq \\ &= -\frac{1}{2\pi i} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^\infty \frac{f(q)}{q - p + i\varepsilon} dq \\ &= -\frac{1}{2\pi i} \left\{ PV \int_{-\infty}^\infty \frac{f(q)}{q - p} dq - i\pi f(p) \right\} \\ &= \frac{1}{2i} (Hf)(p) + \frac{f(p)}{2}. \end{aligned} \quad (2.36)$$

Hence, we have

$$\mathcal{F} \vartheta \mathcal{F}^{-1} = \frac{1}{2} (-iH + \mathbb{I}). \quad (2.37)$$

Now consider the backflow operator defined as  $B = U \mathcal{F} \vartheta \mathcal{F}^{-1} U^* - U^* \mathcal{F} \vartheta \mathcal{F}^{-1} U$ , where  $U = U_{T=1}$  is the unitary evolution operator in the momentum space defined in Eq. (2.16). Substituting (2.37) into the last equation, we obtain

$$B = \frac{1}{2i} (U H U^* - U^* H U). \quad (2.38)$$

From this we have for  $p > 0$  and  $\phi \in \mathcal{S}(\mathbb{R}_+)$

$$\begin{aligned} (\vartheta B \vartheta \phi)(p) &= \frac{e^{-ip^2}}{2i} (H U^* \phi)(p) - \frac{e^{ip^2}}{2i} (H U \phi)(p) \\ &= \frac{1}{2\pi i} \int_0^\infty \frac{e^{-(p^2 - q^2)} - e^{i(p^2 - q^2)}}{p - q} \phi(q) dq \\ &= -\frac{1}{\pi} \int_0^\infty \frac{\sin(p^2 - q^2)}{p - q} \phi(q) dq = (K\phi)(p). \end{aligned} \quad (2.39)$$

Thus the restriction of  $\vartheta B \vartheta \phi$  to  $L^2(\mathbb{R}_+)$  is equal to  $K$ . ■

With the last proposition we proved that searching the maximum amount of backflow for any right-movers is equivalent to finding the supremum element of the spectrum of an integral operator. Furthermore, we have that for a generic right-mover  $\psi = E_+\psi$  with  $\|\psi\| = 1$

$$L(\psi_{t=0}) - L(\psi_{t=1}) = (\hat{\psi}|K\hat{\psi}), \quad (2.40)$$

where  $L(\psi_t)$  is the probability of finding the particle in  $x > 0$  at the time  $t$ .

Following, we discuss some numerical methods to evaluate the backflow constant  $\lambda$  and the wave-function corresponding to maximum backflow.

### 2.3.2 Maximum Backflow Approximation

As we have proved in the Theorem 2.3.4, there exist a lower bound for backflow; in the sense that for every time interval  $[0, T)$  the maximum amount of probability which could flow back for a generic right-mover is always less than  $|\lambda|$ . But we know nothing about  $\lambda$  and its (maybe improper) eigenfunction  $\phi_\lambda$ . In order to evaluate this quantities we need to study the integral operator  $K$ . Unfortunately, It has not been possible to find  $\sup \sigma(K)$  analytically, and numerical methods have been used to estimate  $\lambda$ .

More precisely, we approximate the quarter of Cartesian plane  $(0, \infty)^2$  where the kernel  $\sin(u^2 - v^2)/(u - v)$  is defined by  $[0, N\tau] \times [0, N\tau]$ , divided into a grid of  $N^2$  squares of area  $\tau^2$ . range of integration by the interval  $[0, N\tau]$ . In each square we approximate the kernel of the integral operator as a constant. At the same time we approximate the possible eigenfunction  $\phi_\lambda$  to a vector  $\varphi_\lambda^i$  in  $\mathbb{R}^n$  simply by considering the function constant in each interval  $[i\tau, (i+1)\tau]$  with  $i = 1, \dots, n$ . In this way we are converting our eigenvalue-problem to a linear equation:

$$\frac{1}{\pi} \int_0^\infty \frac{\sin(u^2 - v^2)}{u - v} \varphi(v) dv = \lambda \varphi(u) \xrightarrow{\approx} K_k^i \varphi_\lambda^k = \lambda \varphi_\lambda^i, \quad (2.41)$$

where  $K_k^i$  is the hermitian matrix obtained by approximating our integral kernel. The second equation has surely solution and there exists lots of algorithm that can find the lowest eigenvalue. In order to find a good estimate of our true  $\lambda$  we only need to take  $N \rightarrow \infty$  and  $\tau \rightarrow 0$ . Here we report some results obtained by Braken and Melloy in their work considering  $\tau = 0.05$ . The estimates obtained are:

$N$	$\lambda$
100	-0.0256
200	-0.0297
275	-0.0309
500	-0.0323

which are apparently converging to  $\lambda_{0.05} \approx 0.034$ . Taking smaller values of  $\tau$  and letting  $N \rightarrow \infty$  we can obtain the estimates  $\lambda_{0.04} \approx 0.035$ ,  $\lambda_{0.025} \approx 0.036$  and  $\lambda_{0.01} \approx 0.038$ .

A possible method to compute the maximum eigenvalue  $\lambda$  is given by Penz in [10]. It is based on an algorithm called *power iteration* and works as follows.

Let  $A \in \mathbb{C}^{N \times N}$  be a symmetric matrix and  $a$  the eigenvalue of  $A$  with the largest absolute value. Then, consider a vector  $v_0 \in \mathbb{C}^N$  such that  $v_0 \neq 0$  and there is a non-zero component within the eigenspace of  $A$  corresponding to  $a$ . Then the sequence  $\{v_n\}_{n \in \mathbb{N}_k}$  recursively defined by

$$v_{n+1} = \frac{Av_n}{\|v_n\|} \quad (2.42)$$

converges to a normalized eigenvector of  $a$  and also holds

$$a = \lim_{n \rightarrow \infty} v_{n+1}^\dagger \frac{v_n}{\|v_n\|}. \quad (2.43)$$

Since  $\sigma(\vartheta B \vartheta) = \sigma(K) \subset [-1, \lambda]$ , the power method can be applied to the non negative, discretized operator  $\vartheta B \vartheta + \mathbb{I}$ . Its largest eigenvalue then approximates  $\lambda + 1$  while the sequence  $v_n$  tends to the maximizing eigenvector.

Penz started his calculations by covering a starting square  $[0, q_0]^2$  with  $N_0$  grid points and then repeated the computations for up to  $N = N_0 h$  grid points and a larger square  $[0, q]^2$  with  $q = q_0 \sqrt{h}$  for  $h = 1, 2$ , etc.. With this methodology, we can at the same time make the covered square to grow and the absolute step size to get smaller. This leads to a sequence of eigenvalues  $\lambda_h$  in function of the factor of accuracy  $h$  which are used to extrapolate to  $h \rightarrow \infty$  and getting an approximation  $\lambda_\infty$  of the backflow constant. The results obtained by Penz are plotted in figure (2.3) and (2.4).

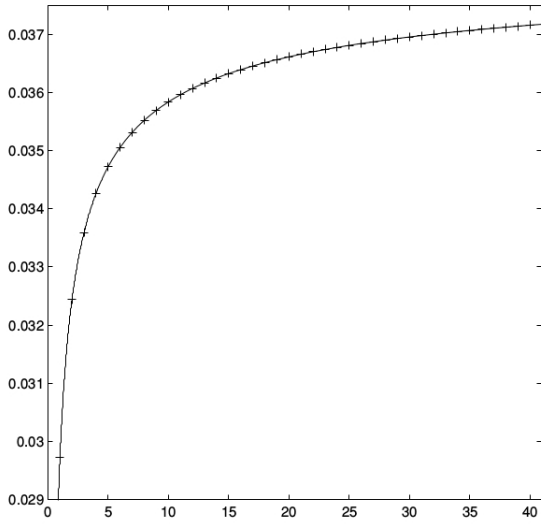


FIGURE 2.3:  $\lambda$  plotted against  $h$  and fit  $\lambda_\infty + b/\sqrt{h}$ .

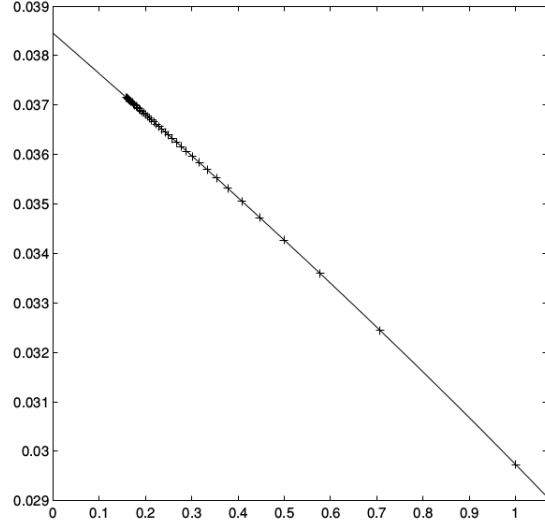


FIGURE 2.4:  $\lambda$  plotted against  $1/\sqrt{h}$  and polynomial fit of third order.

The approximation for the backflow constant can be read off from the intersection of the  $y$ -axis with the graph in (2.4). This yields

$$\lambda \approx \lambda_\infty \approx 0.0384517. \quad (2.44)$$

This is the final result computed by Penz *et al.* in [10]. Another analysis has been done by Eveson, Fewster and Verch in [6] giving an approximation for the backflow constant by  $\lambda \approx 0.038452$ .

## Chapter 3

# Interacting Quantum Backflow

The final chapter will be dedicated to the analysis of backflow in scattering theory. First of all, we will discuss the spatial extension of backflow. We will find that negative probability current could occur on arbitrary large region of space but its average value is bounded from below. After that we will focus on proving the existence of probability backflow also in the presence of a potential  $V(X)$  with some little restricting properties. For this purpose we need to reformulate the concept of right-moving in scattering situation introducing the "interaction picture" of quantum mechanics mentioned in Chapter 1.

The importance of such analysis lies on the fact that the presence of scattering potentials are far more likely than totally free case. If we want to study a possible experimental set-up for observing backflow, we could never be able to cancel all possible potential. Furthermore, since backflow is a really weak phenomenon, also little potentials could interfere strongly with measurements. Hence, a study of backflow in scattering situations is necessary.

In the following discussion, we will retrace mainly Bostelmann's *et al.* work [5] and report their principal results.

### 3.1 Spatially Averaged Backflow

In the last section we investigated some properties of backflow for free right-moving particles focusing in particular above its temporal boundedness. We find out that, no matter how long our wave function is let to evolve, the amount of probability flowing across a reference point given by equation (2.10) is always bigger than a dimensionless constant  $-\lambda \approx 0.038$  for all normalized right-moving wave function. This inequality is a bound on the (averaged) temporal extent of backflow. ~~Up~~ until now, we only studied backflow and the density probability current ~~only~~ on a reference point  $x = 0$ , therefore we want to deepen our knowledge on this phenomenon by studying its (averaged) spatial extension. In particular we want to understand how negative values of  $j_\phi$  could be distributed by considering spatial integrals of the kinematical current. In particular we will find out a lower bound similar to the one we investigated in the previous section. In fact, we will show that:

$$\int_{\mathbb{R}} f(x) j_\phi(x) dx \geq c_f > -\infty \quad (3.1)$$

for all normalized right-movers  $\phi$  and all positive averaging functions  $f \geq 0$ . Here the function  $f$  plays the role of an extended detector, generalizing the step function that we used previously in equation (2.10).

~~But first of all,~~ we report an interesting result obtained by Bostelmann, Cadamuro and Lechner [5] about the possible values of the density current  $j_\phi$  for a normalized right-moving wave function

$\phi$  evaluated in some point  $x \in \mathbb{R}$  (i.e. the origin). We will prove that **for any** this quantity can be arbitrary large.

**3.1.1 Proposition (Unboundedness of  $j_\phi$ ).** *Let  $x \in \mathbb{R}$ . Then there exist sequences  $\phi_n^\pm \in E_+(L^2(\mathbb{R}))$  of right-moving wave functions such that*

$$\lim_{n \rightarrow \infty} j_{\phi_n^\pm}(x) = \pm\infty, \quad (3.2)$$

and the norms  $\|\phi_n^\pm\|_{L^2}^2$  and  $\|\widehat{\phi}_n^\pm\|_{L^1}$  are independent of  $n$ .

*Proof.* Let's start with the construction of the sequence  $\phi_n^+$ . The unboundedness from above is an high-momentum effect, so we need only to select a right-moving wave function  $\phi^+ \in L^2(\mathbb{R})$  such that  $\phi = E_+\phi$  and the current  $j_\phi^+(x)$  exists, and shift it to higher and higher momentum,  $\widehat{\phi}_n^+(p) := \widehat{\phi}^+(p - n)$ . Obviously, the norms  $\|\widehat{\phi}_n^+\|_{L^1} = \|\widehat{\phi}^+\|_{L^1}$  and  $\|\phi_n^+\|_{L^2}^2 = \|\phi^+\|_{L^2}^2$ , so they are not dependent of  $n$ . Furthermore, using the relation  $\phi_n^+ = e^{inx}\phi^+$ , we can show that the current  $\phi_n^+$  ~~has to be~~

$$j_{\phi_n^+}(x) = j_{\phi^+}(x) + n|\phi^+(x)|^2, \quad (3.3)$$

as can be checked on the basis of Equation (1.34). So if the we choose  $\phi^+$  such that  $\phi^+(x) \neq 0$  (which is clearly possible), we find  $\lim_{n \rightarrow \infty} j_{\phi_n^+}(x) = +\infty$ . Now we can prove the unboundedness from below. As we shown in Section 2.2, backflow can be seen as a high-momentum interference effect. So, if we want to construct our negative divergent  $\phi_n^-$  we must use the superposition of a low- and a high-momentum state. We choose a ~~wave~~ function  $\chi$  such that  $\widehat{\chi}$  has compact support on the right-half line and  $\chi(x) \neq 0$ . Such function clearly ~~exist~~ for any  $x$ , and ~~are~~ by construction right-movers. Now we consider the linear combinations  $\widehat{\phi}_n^-(p) := \alpha_n \widehat{\chi}(p) + \beta_n \widehat{\chi}(p - n)$ , where  $n \in \mathbb{N}$ , and  $\{\alpha_n\}, \{\beta_n\} \in \mathbb{C}$  are complex sequences such that  $|\alpha_n| = \alpha$  and  $|\beta_n| = \beta$  are constant. By construction,  $\phi_n^-$  are right-movers and for large  $n$  we have  $\|\phi_n^-\|_{L^2}^2 = (|\alpha|^2 + |\beta|^2)\|\chi\|_{L^2}^2$  and  $\|\widehat{\phi}_n^-\|_{L^1} = (|\alpha| + |\beta|)\|\chi\|_{L^1}$ . At this point, it only remains to choose  $\alpha$  and  $\beta$  in order to have  $\lim_{n \rightarrow \infty} j_{\phi_n^-}(x) = -\infty$ . With this purpose, we can evaluate  $j_{\phi_n^-}(x)$  obtaining:

$$j_{\phi_n^-}(x) = \begin{pmatrix} \alpha^* \\ \beta^* \end{pmatrix}^t [j_\chi(x)\mathbb{I} + nA_n] \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \quad (3.4)$$

where

$$A_n := \begin{bmatrix} 0 & e^{inx} \left( \frac{j_\chi(x)}{n} + \frac{|\chi(x)|^2}{2} \right) \\ e^{-inx} \left( \frac{j_\chi(x)}{n} + \frac{|\chi(x)|^2}{2} \right) & |\chi(x)|^2 \end{bmatrix} \quad (3.5)$$

$A_n$  is a  $2 \times 2$  Hermitian matrix, has trace  $|\chi(x)|^2$ , and  $\lim_{n \rightarrow \infty} \det(A_n) = -|\chi(x)|^4/4 < 0$ . Also, the eigenvalues  $\lambda_\pm(n)$  of  $A_n$  converges to  $\lambda_\pm(n) \rightarrow (1 \pm \sqrt{2})|\chi|^2/2$  as  $n \rightarrow \infty$ . Finally, choosing  $\alpha_n$  and  $\beta_n$  as the coordinates of the eigenvector with the negative eigenvalue  $(1 - \sqrt{2})|\chi|^2/2$  (i.e. take  $\alpha_n = 1/(1 - \sqrt{2})$  and  $\beta_n = \exp(-inx)$ ) we can check that  $\lim_{n \rightarrow \infty} j_{\phi_n^-}(x) = -\infty$  because of the explicit factor  $n$  in front of  $A_n$ . ■

**3.1.2 Observation.** Before turning back to the main goal of this section, we note that the density current function  $j_\psi$  ~~could be thought as a quadratic form defined as~~

$$(\psi|J(x)\psi) := j_\psi(x), \quad (3.6)$$

Here  $J(x)$  could be defined as an "improper" operator (as done by Yearsley in [9]) by the equation

$$J(x_0) = \frac{1}{2}[P\delta(X - x_0) + \delta(X - x_0)P], \quad (3.7)$$

where  $\delta(X)$  stays for the *Dirac delta function*.



With the last equation in mind, we can rewrite the spatial averaged density current by a Schwarz class test function  $f \in \mathcal{S}(\mathbb{R})$  as follow:

$$(\phi|J(f)\phi) := \int_{\mathbb{R}} f(x)j_{\phi}(x) dx, \quad (3.8)$$

where  $J(f)$  can be readily checked to be an (unbounded) operator, Hermitian for real  $f$ , and expressible in terms of the position and momentum operator  $(X, P)$  as in the following definition.

**3.1.3 Definition.** Let  $f \in \mathcal{S}(\mathbb{R})$  be a Schwarz function. We define the **density current operator**  $J(f)$  as follow:

$$J(f) = \frac{1}{2}[Pf(X) + f(X)P]. \quad (3.9)$$

**3.1.4 Observation.** Note that if we take the operator  $E_+J(f)E_+$ , this represents nothing more than the averaged current evaluated in right-moving states. The fact that backflow exists is reflected in the fact that the operator  $E_+J(f)E_+$  is not positive. To formulate this concept more rigorously we can introduce the **bottom of the spectrum** of a Hermitian operator  $A$  defined by

$$\inf(A) := \inf_{\|\phi\|=1} (\phi|A\phi) \in [-\infty, +\infty). \quad (3.10)$$

Then the maximal amount of backflow, spatially averaged by  $f$ , is defined as

$$\beta_0(f) = \inf(E_+J(f)E_+) \quad (3.11)$$

This is completely similar to what done in Chapter 2 where we defined the constant backflow  $\lambda$  as the infimum of a bounded and self-adjoint operator  $B$ .

Now we can enunciate the next Theorem in which we summarize three fundamental properties of the operator  $J(f)$ . The first one is the *existence* of backflow showing that  $\beta_0(f) < 0$  for each positive test function  $f$  (and more strongly for each function  $f \neq 0$ ). The second property is the unboundedness of  $E_+J(f)E_+$  from above that will be proved similarly to the Proposition 3.1.1. The final point regards the existence of an lower bound for our averaged current operator. In fact it will be proved that  $\beta_0(f) > -\infty$ , in contrast with the last Proposition where  $j_{\phi}(x)$  has been proven to be unbounded. In particular, in this part we will recall a result obtained by Eveson, Fewster, and Verch [note] about an interesting relation for  $\beta_0(f)$  with  $f = g^2$ .

**3.1.5 Theorem (Existence and boundedness of spatially averaged Backflow).** In the context of quantum backflow, the following proposition are real:

- (a) For any real  $f \in \mathcal{S}(\mathbb{R})$  with  $f \neq 0$ , the smeared probability flow in right-moving states,  $E_+J(f)E_+$ , is not positive,  $\beta_0(f) < 0$ .
- (b) Let  $f > 0$ . Then there is no finite upper bound on  $E_+J(f)E_+$ .
- (c) Let  $f > 0$ . Then  $E_+J(f)E_+$ , is bounded below, i.e.  $\beta_0(f) > -\infty$ . Furthermore, for any test functions of the form  $f = g^2$  for some real  $g \in \mathcal{S}(\mathbb{R})$ , one has

$$\beta_0(g^2) \geq -\frac{1}{8\pi} \int_{\mathbb{R}} |g'(x)|^2 dx > -\infty. \quad (3.12)$$

*Proof.* (a) First of all, we consider the operator  $E_+J(f)E_+$  and a general function  $\phi \in L^2(\mathbb{R})$ , then considering the Fourier transform of  $E_+J(f)E_+$  we can find out that  $E_+J(f)E_+$  can be thought in the momentum space as an integral operator with his kernel  $K_f$ . In detail we have

$$\begin{aligned} \mathcal{F}E_+J(f)E_+\phi &= \mathcal{F}\mathcal{F}^{-1}\mathcal{F}E_+J(f)\mathcal{F}^{-1}\mathcal{F}E_+\phi = \vartheta(q)\mathcal{F}J(f)\mathcal{F}^{-1}\vartheta(p)\widehat{\phi}(p) = \\ &= \frac{1}{2}\mathcal{F}f(x)\mathcal{F}^{-1}(p+q)\vartheta(q)\vartheta(p)\widehat{\phi}(p) = \int_{-\infty}^{\infty} dp \frac{p+q}{2\sqrt{2\pi}}\widehat{f}(q-p)\vartheta(p)\vartheta(q)\widehat{\phi}(p). \end{aligned} \quad (3.13)$$

Hence we have

$$K_f(q, p) = \frac{p+q}{2\sqrt{2\pi}}\widehat{f}(q-p)\vartheta(p)\vartheta(q), \quad (3.14)$$

but we are considering only right-moving wave function so we can take the restriction of our integral operator to  $L^2(\mathbb{R}_+, dp)$  and neglect the Heaviside functions.

If  $E_+J(f)E_+$  is positive, then we would have

$$\int_0^{+\infty} dq \int_0^{+\infty} dp \varphi^*(q)K_f(q, p)\varphi(p) > 0 \quad \forall \varphi \in L^2(\mathbb{R}_+, dp) \quad (3.15)$$

Then if we consider a sequence  $\{g_n\} \in L^2_0(\mathbb{R})$  of functions converging to the Dirac delta distribution  $\delta_0$ , and two complex numbers  $\alpha$  and  $\beta$ , we must have

$$\int_0^{+\infty} dq' \int_0^{+\infty} dp' [\alpha^*g_n^*(q'-q) + \beta^*g_n^*(q'-p)]K_f(q', p')[\alpha g_n(q'-q) + \beta g_n(q'-p)] > 0, \quad (3.16)$$

for all  $n \in \mathbb{N}$ ,  $\alpha, \beta \in \mathbb{C}$ , and  $p, q > 0$ . So, taking the limit  $n \rightarrow \infty$  we obtain that

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix}^\dagger \begin{bmatrix} K_f(q, q) & K_f(q, p) \\ K_f(q, p) & K_f(p, p) \end{bmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} > 0 \quad \forall \alpha, \beta \in \mathbb{C}, \quad \forall p, q > 0. \quad (3.17)$$

In this paragraph we have proved that the positiveness of the operator  $E_+J(f)E_+$  implies the positiveness of the Hermitian  $2 \times 2$  matrix defined in equation (3.17) for each choice of positive  $p, q$ . In order to be positive, this matrix must have only non-negative eigenvalues, and in particular a non-negative determinant:

$$0 \leq K_f(q, q)K_f(p, p) - |K_f(q, p)|^2 = \frac{pq}{2\pi}|\widehat{f}(0)|^2 - \frac{(p+q)^2}{8\pi}|\widehat{f}(q-p)|^2. \quad (3.18)$$

This implies

$$|\widehat{f}(q-p)| \leq \frac{2\sqrt{pq}}{p+q}|\widehat{f}(0)|. \quad (3.19)$$

Now we can show that, taking  $q \rightarrow 0$  at fixed  $p > 0$ ,  $|\widehat{f}(-p)| = 0$  for all  $p > 0$ . But since  $f$  is real,  $\widehat{f}(-p) = \widehat{f}^*(p)$ , so that  $\widehat{f}(p) = 0$  for each  $p \neq 0$ . As the test function  $f$  is continuous, this implies that  $f = 0$  ~~vanish altogether~~. So we conclude that for any real  $f \neq 0$  the operator  $E_+J(f)E_+$  is not positive.

(b) The proof of this point is ~~pretty~~ similar to the one on Proposition 3.1.1. In fact, we take a normalized right-moving function  $\phi = E_+\phi \in L^2(\mathbb{R})$ , and define a sequence of shifted-momentum wave functions  $\widehat{\phi}_n(p) = \widehat{\phi}(p-n)$  with  $n \in \mathbb{N}$ . It's obvious that  $\|\phi_n\|_{L^2} = 1$  and  $E_+\phi_n = \phi_n$ . Furthermore, the expectation value of  $E_+J(f)E_+$  is

$$(\phi_n|E_+J(f)E_+\phi_n) = (\phi|E_+J(f)E_+\phi) + n \int_{-\infty}^{+\infty} f(x)|\phi(x)|^2 dx. \quad (3.20)$$

For  $f > 0$ , it is clear that there exist  $\phi$  such that the last integral is positive and in this case we have  $\lim_{n \rightarrow \infty} (\phi_n | E_+ J(f) E_+ \phi_n) = +\infty$ , showing that the operator  $E_+ J(f) E_+$  has no finite upper bound.

(c) In order to prove the final thesis of this theorem, we consider a general normalized right-moving function  $\phi = E_+ \phi \in L^2(\mathbb{R})$  and a general real function  $g \in \mathcal{S}(\mathbb{R})$  and consider the averaged spaced density current

$$\begin{aligned} (\phi | E_+ J(g^2) E_+ \phi) &= \operatorname{Re}(\phi | g^2(X) P \phi) \\ &= \operatorname{Re}[(\phi | g(X) P g(X) \phi) + (\phi | g(X) [g(X), P] \phi)] \\ &= \operatorname{Re}[(\phi | g(X) P g(X) \phi) + i(\phi | g(X) g'(X) \phi)] \\ &= \operatorname{Re}(\phi | g(X) P g(X) \phi) = (g(X) \phi | P g(X) \phi) \\ &= \int_{-\infty}^{+\infty} p |\mathcal{F}[g(X) \phi](p)|^2 dp. \end{aligned} \quad (3.21)$$

Where  $[g(X), P]$  is the commutator between the multiplication operator  $g(X)$  and the differential operator  $P$ , which is known to be  $ig'(X)$ . We therefore may obtain a bound by considering only the integral only on  $(-\infty, 0)$ :

$$(\phi | E_+ J(g^2) E_+ \phi) \geq \int_{-\infty}^0 p |\mathcal{F}[g(X) \phi](p)|^2 dp = - \int_0^{\infty} p |\mathcal{F}[g(X) \phi](-p)|^2 dp. \quad (3.22)$$

By the Convolution Theorem we can rewrite  $\mathcal{F}[g(X) \phi]$  as

$$\mathcal{F}[g(X) \phi](p) = \frac{1}{\sqrt{2\pi}} \int_0^{\infty} dp' \hat{\phi}(p') \hat{g}(p - p'), \quad (3.23)$$

where the restriction  $p' > 0$  rise immediately from  $E_+ \phi = \phi$ . Now applying the Cauchy-Schwarz Theorem, we obtain:

$$\begin{aligned} |\mathcal{F}[g(X) \phi](-p)|^2 &= \left| \frac{1}{\sqrt{2\pi}} \int_0^{\infty} dp' \hat{\phi}(p') \hat{g}(-p - p') \right|^2 \leq \frac{\|\phi\|^2}{2\pi} \int_0^{\infty} dp' |\hat{g}(-p - p')|^2 = \\ &= \frac{1}{2\pi} \int_0^{\infty} dp' |\hat{g}(p + p')|^2, \end{aligned} \quad (3.24)$$

where we have also used  $|\hat{g}(-p)|^2 = |\hat{g}(p)|^2$  (since  $g$  is real) and  $\|\phi\| = 1$ . Substituting into equation (3.22), we can calculate:

$$\begin{aligned} (\phi | E_+ J(g^2) E_+ \phi) &\geq - \frac{1}{2\pi} \int_0^{\infty} dp \int_0^{\infty} dp' p |\hat{g}(p + p')|^2 \\ &= - \frac{1}{2\pi} \int_0^{\infty} du |\hat{g}(u)|^2 \int_0^u dp p \\ &= - \frac{1}{4\pi} \int_0^{\infty} du u^2 |\hat{g}(u)|^2 \\ &= - \frac{1}{8\pi} \int_{-\infty}^{\infty} du u^2 |\hat{g}(u)|^2 \\ &= - \frac{1}{8\pi} \int_{-\infty}^{\infty} dx |g'(x)|^2 \quad \forall \phi \in L^2(\mathbb{R}), \end{aligned} \quad (3.25)$$

where we have changed the variables  $(p, p')$  to  $(u, p)$  with  $u = p + p'$ , used evenness of  $|\hat{g}(u)|^2$  and Parseval's Theorem. This last equation complete the proof of the inequality (3.12). This also

proves the boundedness of  $E_+J(f)E_+$  for all Schwarz functions  $f > 0$  since there always exists a another  $g \in \mathcal{S}(\mathbb{R})$  such that  $g^2 = f$ . ■

Until now, we considered right-moving functions at a fixed time and no assumption on potentials are made yet. In the following section we start the analysis of backflow in scattering theory by introducing the concept of *interacting state* and *asymptotic solutions* of Schrödinger equation.

## 3.2 Backflow and Scattering

Let us consider physical system described by the Hamiltonian of the form  $H = \frac{1}{2}P^2 + V(X)$ , where  $V(X)$  is a general time-independent potential described as a function of the position  $X$ . We want to answer the question if backflow could occur and if there exists a lower bound for the averaged spatial density current. The first conceptual problem that we encounter is that in non-zero potential situation, the space of right-movers  $E_+(L^2(\mathbb{R}))$  is no longer invariant under time evolution. Hence, it's more difficult to define when a particle travels to the right. To overcome this, we can substitute the concept of right-moving solutions with the "asymptotic momentum" distributions in the sense of scattering theory. It consists on those kind of solutions such that for  $t \rightarrow -\infty$  (when the particle is still far away from the potential zone) are right-movers in the usual sense. This space has the property to be invariant under time evolution and describes particles scattering "from the left" onto the potential. We can ask ourself where is the connection between the asymptotic state  $\psi$  and the "interacting state"  $\Omega_V\psi$ . The answer is given by the Møller operator defined as:

$$\Omega_V := \lim_{t \rightarrow -\infty} e^{iHt} e^{-iH_0 t}, \quad (3.26)$$

where  $H_0$  means the free Hamiltonian  $P^2/2$ . As just mentioned in Chapter 1 the last equation has to be read in this way: Given a fixed wave-function at time  $t = 0$ , we want to find what would have been the particle state if it had evolved from  $t \rightarrow -\infty$  until  $t = 0$  under the evolution operator defined by the interacting Hamiltonian  $H$ . For this purpose, we have to evolve our input state backwards in time until some  $t < 0$ . Then we pull forward the time but now using the interacting Hamiltonian. We repeat this process taking  $t \rightarrow -\infty$ . We remark that, although  $\Omega_V$  is not unitary in the presence of bound states, we still have  $\|\Omega_V\| = 1$ .

As mentioned before, We will now look at the averaged probability current  $J(f)$  in asymptotically right-moving states. Thus, we consider the "asymptotic current operator" defined as

**3.2.1 Definition.** Let  $J(f)$  be the density current operator defined in Eq. (3.9),  $E_+$  the orthogonal projector in right-movers space and  $\Omega_V$  the Møller operator. We call the **asymptotic current operator**

$$E_+ \Omega_V^* J(f) \Omega_V E_+. \quad (3.27)$$

**3.2.2 Remark.** The goal of this section is to investigate the spectral properties of this operator - whether it is unbounded above (unlimited forward flow) or bounded below (limited backflow) - and how to estimate the *backflow constant*:

$$\beta_V(f) := \inf(E_+ \Omega_V^* J(f) \Omega_V E_+). \quad (3.28)$$

In order to be able to do scattering theory, we need to impose our potentials  $V(x)$  to be sufficiently fast decreasing as  $x \rightarrow \pm\infty$ . Hence we have the following definition.

**3.2.3 Definition.** We define  $L^{1+}(\mathbb{R})$  the set of all real functions  $V$  such that the norm

$$\|V\|_{1+} := \int_{-\infty}^{\infty} (1 + |x|)|V(x)| dx < \infty \quad (3.29)$$

exists finite.

**3.2.4 Observation.** Taking potentials in  $L^{1+}$ , the time-independent Schrödinger equation for scattering states is of the form:

$$[-\partial_x^2 + 2V(x) - k^2]\psi(x) = 0 \quad k \in \mathbb{R}. \quad (3.30)$$

In stationary picture of scattering theory, we are particularly interested on solutions  $\varphi_k$ ,  $k > 0$ , of Eq. (3.30) with the following asymptotics:

$$\varphi_k(x) = \begin{cases} T_V(k)e^{ikx} + o(1) & \text{for } x \rightarrow +\infty \\ e^{ikx} + R_V(k)e^{-ikx} + o(1) & \text{for } x \rightarrow -\infty \end{cases} \quad (3.31)$$

where  $R_V(k)$  and  $T_V(k)$  denote the reflection and transmission coefficients of the potential  $V$ , respectively. What we are doing here is to choose all those kind of solutions that behave like plane waves which scatter against a potential wall, resulting into a transmitted plane wave  $e^{ikx}T_V(k)$  and into a reflected wave  $R_V(k)e^{-ikx}$  (See Fig. (3.2)).

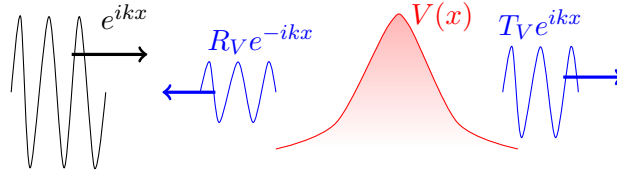


FIGURE 3.1: Sketch of a scattering process of a plane wave with momentum  $k$  into a potential  $V(x)$  resulting into reflected and transmitted waves as Eq. (3.31)

At this point, we shall recall some important results of scattering theory in this context. A deeper and more exhaustive analysis of mathematical aspects of scattering theory could be found in [12].

**3.2.5 Lemma.** Let  $V \in L^{1+}$ . Then the Møller operator  $\Omega_V$  exists. Furthermore, the solution  $x \mapsto \varphi_k(x)$  ( $k > 0$ ) of Eq. (3.30) with the asymptotic conditions of Eq. (3.31) exists and is unique, and for any  $\hat{\psi} \in C_0^\infty(\mathbb{R})$

$$(\Omega_V E_+ \psi)(x) = \frac{1}{\sqrt{2\pi}} \int_0^\infty \varphi_k(x) \hat{\psi}(k) dk. \quad (3.32)$$

We will stick to report the references where finding an exhaustive proof of this lemma. Existence and uniqueness of solution  $\varphi_k$  are just consequence of [12, Chap. 5, Lemma 1.1]. Existence of  $\Omega_V$  (under weaker assumption on  $V$ ) can be found also in [12, Chap. 5, Theorem 1.12].

**3.2.6 Observation.** Let us dwell a little on the meaning of Eq. (3.32). What we are doing here is considering a smooth wave-function  $\psi$  with momentum representation  $\hat{\psi} \in C_0^\infty(\mathbb{R})$ . First of all, we remark our interest only in "right moving" solutions. Then, we will not consider the function  $\hat{\psi}(k)$  for  $k < 0$ . Considering only the "right moving" components of  $\psi$  we can thought of them

as independent plane wave functions  $e^{ikx}\widehat{\psi}(k)$  (parametrized in  $k > 0$ ) which scatter into the potential  $V$  giving the solutions  $\varphi_k$ . In the end, we just sum up all the interacting components in order to find out the solution  $\Omega_V E_+ \psi$ .

**3.2.7 Remark.** From here after, we will consider only wave functions  $\psi$  such that  $\widehat{(\psi)} \in C_0^\infty(\mathbb{R})$  as in Lemma 3.2.5 in order to have a well defined asymptotic current operator  $E_+ \Omega_V^* J(f) \Omega_V E_+$ . This is not a big issue since such a space could be proved to be dense in  $L^2(\mathbb{R})$ .

**3.2.8 Observation.** Using Eq. (3.32), we are able to estimate the expectation values of the asymptotic current operator as follow

$$(\psi | E_+ \Omega_V^* J(f) \Omega_V E_+ \psi) = \int_{-\infty}^{\infty} dx f(x) \int_0^{\infty} dp \int_0^{\infty} dq \widehat{\psi}^*(p) K_V(p, q, x) \widehat{\psi}(q), \quad (3.33)$$

where  $K_V$  is defined as

$$K_V(p, q, x) = \frac{i}{4\pi} [\partial_x \varphi_p^*(x) \varphi_q(x) - \varphi_p^*(x) \partial_x \varphi_q(x)]. \quad (3.34)$$

Retracing the work of Bostelmann *et al.* [5], the next step of our analysis is to give some important bounds on the solution  $\varphi_k$  and  $K_V$  relating them to their spatial asymptotics. As in the previous lemma, we will not give any proof of those bounds, but we will just cite the references where this lemma is taken from.

**3.2.9 Lemma.** Let  $V \in L^{1+}(\mathbb{R})$ ,  $\varphi_k$  (with  $k > 0$ ) is the solution of (3.30) with the asymptotics (3.31), and  $K_V$  the function defined in (3.34). Then, there exist constants  $c_V, c'_V, c''_V, c'''_V > 0$  such that for all  $x \in \mathbb{R}$  and  $p, q, k > 0$

$$|\varphi_k(x)| \leq c_V(1 + |x|), \quad (3.35)$$

$$|\varphi_k(x) e^{ikx}| \leq c'_V \frac{1 + |x|}{1 + k}, \quad (3.36)$$

$$|\partial_x \varphi_k(x) - ik \varphi_k(x)| \leq c''_V \frac{1}{1 + k}, \quad (3.37)$$

$$\left| K_V(p, q, x) - \frac{p + q}{4\pi} \varphi_p^*(x) \varphi_q(x) \right| \leq c'''_V(1 + |x|). \quad (3.38)$$

The first two bounds in Eqs. (3.35) and (3.36) can be deduced from [13, Sec. 2, Lemma 1], paying attention on the fact that the function  $m(x, k)$  there corresponds to our  $\varphi_k(x) e^{-ikx} / T_V(k)$ , while  $T_V(k)$  is taken such that  $|T_V(k)| \leq 1$  and  $T_V(k) = 1 + O(1/k)$  for large  $k$  [13, Sec. 2, Theorem 1]. The last two bounds in Eqs. (3.37) and (3.38) are consequence of (3.35) and (3.36). The constants  $c_V, c'_V, c''_V$ , and  $c'''_V$  can be deduced from [13] as functions of  $V$ , although they are not optimal and we will not use them during the following discussion. With these informations in mind, we have arrived to the first main result for backflow in scattering theory. We will prove the unboundedness of asymptotic current operator  $E_+ \Omega_V^* J(f) \Omega_V E_+$  and existence of backflow as the presence of negative parts of the spectrum, generalizing the results of the free situation (see Th. 3.1.5).

**3.2.10 Theorem (Existence of backflow in scattering situations).** Let  $V \in L^{1+}(\mathbb{R})$ . Then,

- (a) for every  $f \in \mathcal{S}(\mathbb{R})$  with  $f > 0$ , There is no finite upper bound on the asymptotic current operator  $E_+ \Omega_V^* J(f) \Omega_V E_+$ ,
- (b) for every  $x \in \mathbb{R}$ , there is a sequence of normalized right-movers  $\psi_n = E_+ \psi_n$  such that  $\lim_{n \rightarrow \infty} (\psi_n | \Omega_V^* J(x) \Omega_V \psi_n) = -\infty$ .

**3.2.11 Observation.** ~~Before giving the proof to Theorem 3.2.10, let us note that point (b) means that the backflow constant  $\beta_V(f)$  could be negative for some positive  $f$ , thus averaged backflow exists in all scattering situations. The difference with the free case is that  $\beta_0(f)$  has proved in Th. 3.1.5 to be negative for all positive Schwarz functions  $f$ . In scattering situations, we are not able to give an analogous statement for  $\beta_V(f)$ .~~

*Proof of Theorem 3.2.10.* (a). To proof the unboundedness of  $E_+\Omega_V^*J(f)\Omega_VE_+$ , ~~we recover what done in Theorem 3.1.5 (b). Hence, we consider a right-mover  $\psi = E_+\psi$  such that  $\hat{\psi} \in C_0^\infty(\mathbb{R}_+)$  (unless the current operator could not be defined) and shift it to higher momentum defining the sequence  $\psi_n(p) := \hat{\psi}(p-n)$ . In view of the unboundedness of  $(\psi_n|E_+J(f)E_+\psi_n)$  from above [as in Theorem 3.1.5(b)], we only need to show that the sequence  $(\psi_n|(\Omega_V^*J(f)\Omega_V - J(f))\psi_n)$  is bounded as  $n \rightarrow \infty$ . In fact, from Eq. (3.33) we have~~

$$\begin{aligned} (\psi_n|(\Omega_V^*J(f)\Omega_V - J(f))\psi_n) &= \int_{-\infty}^{\infty} dx f(x) \int_{\mathbb{R}_+^2} dp dq \times \\ &\times \left\{ \hat{\psi}_n^*(p)\hat{\psi}_n(q) \left[ K_V(p, q, x) - \frac{p+q}{4\pi} \varphi_p^*(x)\varphi_q(x) \right] + \right. \\ &\left. + \hat{\psi}^*(p)\hat{\psi}(q) \frac{p+q+2n}{4\pi} \left[ \varphi_{p+n}^*(x)\varphi_{q+n}(x) - e^{i(q-p)x} \right] \right\}, \end{aligned} \quad (3.39)$$

where  $\varphi$  are the usual solutions of Lemma 3.2.5. Since the norms  $\|\hat{\psi}_n\|_{L^1}$  are independent of  $n$ , the first summand is bounded in view of Eq. (3.38). Eqs. (3.35) and (3.36) yield the same for the second summand. This proves point (a).

(b) Non-positiveness of asymptotic current operator  $E_+\Omega_V^*J(f)\Omega_VE_+$  could be proved similarly. Here we take a sequence of right-movers  $\psi_n^-$  as in Prop. 3.1.1. Then, it suffices to show that  $(\psi_n|(\Omega_V^*J(f)\Omega_V - J(x))\psi_n)$  is bounded in the same way of point (a), using a suitable choice of  $\chi$  (such that  $\hat{\chi} \in C_0^\infty(\mathbb{R}_+)$ ) as in Prop. 3.1.1. ■

Now, ~~we are ready for the main result of this chapter: the boundedness of the backflow constant  $\beta_V(f)$  for every fixed non-negative Schwarz test-function  $f$  and with potential  $V \in L^{1+}$ . For this purpose, we need to take the asymptotic current operator  $E_+\Omega_V^*J(f)\Omega_VE_+$  and split it into several terms (see in Observation (3.2.13)).~~

**3.2.12 Observation.** Consider the projector into the "left-movers" space  $E_-$  from Def. 2.2.2 and define the operator  $T_V$  acting by multiplication with the transmission coefficient  $T_v(k)$  from Eq. (3.31) in momentum space. Hence, we have

- (i)  $T_V$  commutes with  $E_\pm$  (i.e.  $E_\pm T_V = T_V E_\pm$ ) and  $E_- T_V E_+ = E_- E_+ T_V = 0$ . The first statement comes from the fact that  $E_\pm$  and  $T_V$  are defined as multiplicative operators in momentum space and the second from the identity  $E_\pm E_\mp = 0$ .
- (ii)  $E_- \Omega_V E_+ = E_- (\Omega_V - T_V) E_+$  as consequence of point (i).

**3.2.13 Observation (Bounds of current operator).** Rewriting the operator  $E_+\Omega_V^*J(f)\Omega_VE_+$  we will use the identity  $E_- + E_+ = \mathbb{I}$  and  $(i+P)^{-1}(i+P) = \mathbb{I}$ . Hence, we obtain

$$\begin{aligned} E_+\Omega_V^*J(f)\Omega_VE_+ &= E_+\Omega_V^*(E_- + E_+)J(f)(E_- + E_+)\Omega_VE_+ \\ &= E_+\Omega_V^*E_+J(f)E_+\Omega_VE_+ \\ &\quad + E_+\Omega_V^*E_+J(f)(i+P)^{-1}E_-(i+P)(\Omega_V - T_V)E_+ \\ &\quad + E_+(\Omega_V^* - T_V^*)(-i+P)E_-(-i+P)^{-1}J(f)\Omega_VE_+. \end{aligned} \quad (3.40)$$

Here we used the results from Oss. 3.2.12, the commutativity between  $(i+P)$  and  $E_\pm$  and the adjoint  $(i+P)^* = (-i+P)$ . Note that the first term on the right side in Eq. (3.40) is bounded



by the constant  $\beta_0(f)$  (as proved in Theorem 3.1.5) and  $\|E_+\| = \|\Omega_V\| = 1$ .

Proceeding with analysis of Bostelmann's *et al.* work, we must evaluate the other terms on the right of Eq. (3.40) in order to prove the existence of maximum backflow. In particular we want show that

$$\begin{aligned} \inf(E_+\Omega_V^*J(f)\Omega_VE_+) &\geq \beta_0(f) - 2\|J(f)(i+P)^{-1}\|\|(i+P)(\Omega_V - T_V)E_+\| \\ &\geq \beta_0(f) - 2\|J(f)(i+P)^{-1}\|[2 + \|P(\Omega_V - T_V)E_+\|], \end{aligned} \quad (3.41)$$

where the norms  $\|J(f)(i+P)^{-1}\|$  and  $\|P(\Omega_V - T_V)E_+\|$  are need to be proved to be finite.

In order to estimate  $\|J(f)(i+P)^{-1}\|$ , it will be useful to introduce the concept of Green's function. The Green's function (or fundamental solution) of a linear differential operator  $L$  is defined as ~~that~~ distribution  $G$  such that  $LG = \delta$ , where  $\delta$  is the Dirac's delta function. Such a distribution is useful to find general solution of the differential equation  $Lu = f$ . In fact, such solution  $u$  could be write as  $u = G \star f$ . Since  $L$  is a differential operator, it could act only on the Green's function giving  $L(G \star f) = LG \star f = \delta \star f = f$ . In our case, we are interested in finding the Green's function of the Schrödinger equation.

**3.2.14 Proposition.** Consider the function  $G_k(x)$  defined as

$$G_k(x) := \frac{\sin(kx)}{k} \vartheta(x). \quad (3.42)$$

Then,  $G_k$  is the solution of equation  $-G_k''(x) = k^2 G_k(x) - \delta(x)$  in the sense of distributions, i.e.  $G_k$  is the fundamental solution of the ~~Schrödinger equation~~.

The solution  $\varphi_k$  of Eq. (3.30) could be uniquely determined using  $G_k$  by the following integral equation (Lippman-Schwinger equation)

$$\varphi_k(x) = T_V(k)e^{ikx} + \int_{-\infty}^{\infty} 2V(y)G_k(y-x)\varphi_k(y) dy, \quad (3.43)$$

where the ~~integral means nothing more than the~~ convolution product between  $G_k$  and  $\varphi_k \cdot V$ . With this information at hand, we can prove the following proposition.

**3.2.15 Proposition.** Let  $V \in L^{1+}(\mathbb{R})$ . Then

$$\|P(\Omega_V - T_V)E_+\| \leq 2c_V\|V\|_{1+} \quad (3.44)$$

with the constant  $c_V$  from Lemma 3.2.9.

*Proof.* Consider  $\xi, \psi$  such that  $\hat{\xi}, \hat{\psi} \in C_0^\infty(\mathbb{R})$  and  $\psi = E_+\psi$ . Lemma 3.2.5 gives us

$$\begin{aligned} (\xi|P(\Omega_V - T_V)\psi) &= (P\xi|(\Omega_V - T_V)\psi) \\ &= \frac{i}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \xi^*(x) \int_0^{\infty} dk [\varphi_k(x) - T_V(k)e^{ikx}] \hat{\psi}(k). \end{aligned} \quad (3.45)$$

The expression above may be rewritten in view of Eq. (3.43) and using Fubini's theorem and integration by parts. Thus, we obtain

$$\begin{aligned} (\xi|P(\Omega_V - T_V)\psi) &= \frac{i}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \xi^*(x) \int_0^{\infty} dk \int_{-\infty}^{\infty} dy 2V(y)G_k(y-x)\varphi_k(y). \\ &= \frac{2i}{\sqrt{2\pi}} \int_{\mathbb{R}^2} dx dy \int_0^{\infty} dk \xi(x)^* V(y) \cos[k(y-x)] \vartheta(y-x)\varphi_k(y)\hat{\psi}(k) \end{aligned} \quad (3.46)$$



Now, we introduce the multiplicative operator  $M_y$  (with  $y \in \mathbb{R}$ ) defined as

$$\mathcal{F}[M_y \psi](k) := \varphi_k(y) \hat{\psi}(k) \quad (3.47)$$

and the integral operator  $I_y$  defined by

$$(I_y \hat{\psi})(x) := \vartheta(y - x) \int_0^\infty \cos[k(y - x)] \hat{\psi}(k) dk. \quad (3.48)$$

As noted in [5, Prop. 2], the last equation consists of a projection onto only the positive and even momentum part of  $\psi$ , a multiple of the Fourier transform, a multiplication by the Heaviside function, and a change of variables  $x \mapsto y - x$ . Thus, we have  $\|I_y\| \leq \sqrt{2\pi}$  for all  $y \in \mathbb{R}$ . Using Lemma 3.2.9 Eq. (3.35), we also evaluate the following bound for  $M_y$ :

$$\|M_y \psi\| \leq (c_V(1 + |y|)) \|\psi\| \Rightarrow \|M_y\| \leq c_V(1 + |y|) \quad \forall y \in \mathbb{R}. \quad (3.49)$$

Substituting the previous bounds in Eq. (3.46), yields

$$\begin{aligned} |(\xi | P(\Omega_V - T_V) \psi)| &\leq \frac{2\|\xi\| \|\psi\|}{\sqrt{2\pi}} \int_{-\infty}^\infty |V(y)| \|I_y\| \|M_y\| dy \\ &\leq 2c_V \|\xi\| \|\psi\| \int_{-\infty}^\infty |V(y)| (1 + |y|) dy \\ &\leq 2c_V \|V\|_{1+} \|\xi\| \|\psi\|. \end{aligned} \quad (3.50)$$

Since  $\xi$  and  $\psi$  are taken respectively from a dense subspace of  $L^2(\mathbb{R})$  and  $E_+ L^2(\mathbb{R})$ , this finishes the proof.  $\blacksquare$

Summing up all the results obtained Obs. (3.2.13), Eq. (3.40), and Prop. 3.2.15, Bostelmann *et al.* arrive at the other main result of their work.

**3.2.16 Theorem (Boundedness of backflow in scattering situations).** *For any potential  $V \in L^{1+}$  and any non-negative  $f \in \mathcal{S}(\mathbb{R})$ , there exists a lower bound on the spatially averaged backflow:*

$$\beta_V(f) \geq \beta_0(f) - [2\|f\|_\infty + \|f'\|_\infty](2 + 2c_V \|V\|_{1+}) > -\infty, \quad (3.51)$$

where  $\|f\|_\infty := \sup_{x \in \mathbb{R}} |f(x)|$ ,  $\beta_0(f)$  is the backflow constant in Th. 3.1.5, and  $c_V$  is the constant from Lemma 3.2.9.

*Proof.* To prove this bound we reconsider Eq. (3.41)

$$\inf(E_+ \Omega_V^* J(f) \Omega_V E_+) \geq \beta_0(f) - 2\|J(f)(i + P)^{-1}\| [2 + \|P(\Omega_V - T_V)E_+\|]. \quad (3.52)$$

As said in the end of Obs. 3.2.13, we must prove the existence of finite bounds for  $\|P(\Omega_V - T_V)E_+\|$  and  $\|J(f)(i + P)^{-1}\|$ . The first one is given by Prop. 3.2.15. To prove that  $\|J(f)(i + P)^{-1}\|$ , we note from the definition of  $J(f)$  in Eq. (3.9) that

$$J(f) = \frac{1}{2}[Pf(X) + f(X)P] = \frac{1}{2}\left[[P, f(X)] + 2f(X)P\right] = f(X)P - \frac{i}{2}f'(X). \quad (3.53)$$

Hence we have  $\|J(f)(i + P)^{-1}\| \leq \|f\|_\infty + \frac{1}{2}\|f'\|_\infty$ . Substituting everything into the first equation (3.52), we have our thesis.  $\blacksquare$

The last Theorem concludes our investigation on the existence of backflow in interacting situation. Retracing the work done by Bostelmann *et al.*, we have shown that the asymptotic current operator  $E_+ \Omega_V^* J(f) \Omega_V E_+$  is bounded from below. Thus, in any scattering situations backflow can occur, but its value spatially averaged under a non-negative test-function  $f$  is always bigger than the constant  $\beta_V(f)$ . Note that Eq. (3.51) says very little about the actual value of this bound and some numerical analysis are need for different types of potentials  $V$ . Some examples are given in [5, Sect. IV].

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